Acetic acid, (2,4-dichlorophenoxy)-, butyl ester

Other names:	2,4-D butyl ester
	2,4-D n-butyl ester
	2,4-DBE
	2,4-Dichlorophenoxyacetic acid butyl ester
	2,4-Dichlorophenoxyacetic acid n-butyl ester
	Butapon
	Butyl (2,4-dichlorophenoxy)acetate
	Butyl 2,4-D
	Butyl dichlorophenoxyacetate
	Butyl ester 2,4-D
	Butyl ester of 2,4-D
	Esso Herbicide 10
	Fernesta
	Hi-Ester 2,4-D
	Lironox
	NSC 409767
	Shell 40
	n-Butylester kyseliny 2,4-dichlorfenoxyoctove
Inchi:	InChI=1S/C12H14Cl2O3/c1-2-3-6-16-12(15)8-17-11-5-4-9(13)7-10(11)14/h4-5,7H,2-3,6,8
InchiKey:	UQMRAFJOBWOFNS-UHFFFAOYSA-N
Formula:	C12H14Cl2O3
SMILES:	CCCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	277.14
CAS:	94-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-219.47	kJ/mol	Joback Method
hf	-485.92	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.715		Crippen Method
mcvol	193.970	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1841.00		NIST Webbook

rinpol	1840.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1841.00		NIST Webbook
ripol	2641.00		NIST Webbook
ripol	2641.00		NIST Webbook
ripol	2641.00		NIST Webbook
tb	684.17	K	Joback Method
tc	897.09	K	Joback Method
tf	430.69	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.35	J/mol×K	897.09	Joback Method
cpg	471.09	J/mol×K	684.17	Joback Method
cpg	483.75	J/mol×K	719.66	Joback Method
cpg	495.64	J/mol×K	755.14	Joback Method
cpg	506.74	J/mol×K	790.63	Joback Method
cpg	517.06	J/mol×K	826.11	Joback Method
cpg	526.59	J/mol×K	861.60	Joback Method
dvisc	0.0001246	Pa×s	684.17	Joback Method
dvisc	0.0008297	Pa×s	430.69	Joback Method
dvisc	0.0005252	Pa×s	472.94	Joback Method
dvisc	0.0003584	Pa×s	515.18	Joback Method
dvisc	0.0002591	Pa×s	557.43	Joback Method
dvisc	0.0001961	Pa×s	599.68	Joback Method
dvisc	0.0001540	Pa×s	641.92	Joback Method
hvapt	76.30	kJ/mol	508.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.15048e+01
Coeff. B	-3.55327e+03

Coeff. C	-1.45060e+02
Temperature range (K), min.	444.00
Temperature range (K), max.	718.79

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94804&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume