

(2,4,5-Trichlorophenoxy)acetic acid, monobutylene glycol ester

Other names: 4-hydroxybutyl (2,4,5-trichlorophenoxy)acetate

Inchi: InChI=1S/C12H13Cl3O4/c13-8-5-10(15)11(6-9(8)14)19-7-12(17)18-4-2-1-3-16/h5-6,16H,

InchiKey: VXWTVROLUSKWJR-UHFFFAOYSA-N

Formula: C12H13Cl3O4

SMILES: O=C(COc1cc(Cl)c(Cl)cc1Cl)OCCCCO

Mol. weight [g/mol]: 327.59

CAS: 40583-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-377.85	kJ/mol	Joback Method
hf	-665.36	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.341		Crippen Method
mcvol	212.080	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	818.76	K	Joback Method
tc	1026.04	K	Joback Method
tf	533.95	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.67	J/molxK	818.76	Joback Method
cpg	548.98	J/molxK	853.31	Joback Method
cpg	557.54	J/molxK	887.85	Joback Method
cpg	565.37	J/molxK	922.40	Joback Method
cpg	572.47	J/molxK	956.95	Joback Method
cpg	578.82	J/molxK	991.49	Joback Method
cpg	584.44	J/molxK	1026.04	Joback Method
dvisc	0.0002723	Paxs	533.95	Joback Method

dvisc	0.0001467	Paxs	581.42	Joback Method
dvisc	0.0000868	Paxs	628.89	Joback Method
dvisc	0.0000553	Paxs	676.36	Joback Method
dvisc	0.0000373	Paxs	723.82	Joback Method
dvisc	0.0000265	Paxs	771.29	Joback Method
dvisc	0.0000195	Paxs	818.76	Joback Method

Sources

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=C40583173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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