Acetic acid, (2,4,5-trichlorophenoxy)-, octyl ester

Other names: Octyl 2-(2,4,5-trichlorophenoxy)acetate
octyl (2,4,5-trichlorophenoxy)acetate
2,4,5-Trichlorophenoxyacetic acid, octyl ester

Inchi: InChI=1S/C16H21Cl3O3/c1-2-3-4-5-6-7-8-21-16(20)11-22-15-10-13(18)12(17)9-14(15)19

InchiKey: VXWISAHTAQYMSH-UHFFFAOYSA-N

Formula: C16H21Cl3O3

SMILES: CCCCCCCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 367.69

CAS: 2630-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-207.35	kJ/mol	Joback Method
hf	-595.69	kJ/mol	Joback Method
hfus	46.64	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.929		Crippen Method
mcvol	262.570	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	818.10	K	Joback Method
tc	1026.39	K	Joback Method
tf	518.21	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.38	J/mol×K	1026.39	Joback Method
cpg	765.83	J/mol×K	991.67	Joback Method
cpg	756.36	J/mol×K	956.96	Joback Method
cpg	745.96	J/mol×K	922.24	Joback Method

cpg	734.61	J/mol×K	887.53	Joback Method
cpg	722.31	J/mol×K	852.81	Joback Method
cpg	709.05	J/mol×K	818.10	Joback Method
dvisc	0.0004467	Pa×s	518.21	Joback Method
dvisc	0.0000661	Pa×s	818.10	Joback Method
dvisc	0.0000820	Pa×s	768.12	Joback Method
dvisc	0.0001047	Pa×s	718.14	Joback Method
dvisc	0.0001387	Pa×s	668.15	Joback Method
dvisc	0.0001923	Pa×s	618.17	Joback Method
dvisc	0.0002824	Pa×s	568.19	Joback Method
hvapt	92.20	kJ/mol	517.50	NIST Webbook

Sources

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=C2630151&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume