2,4,5-Trichlorophenoxyacetic acid, 2-ethylhexyl ester

Other names: Acetic acid, (2,4,5-trichlorophenoxy)-, 2-ethylhexyl ester
2,4,5-T 2-ethylhexyl ester
2-Ethylhexyl 2,4,5-trichlorophenoxyacetate
2,4,5-T Ethyl hexyl ester

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

InchiKey: MNELUOHPQMJXGU-UHFFFAOYSA-N

Formula: C16H21Cl3O3

SMILES: CCCCC(CC)COC(=O)COc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 367.69

CAS: 1928-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-209.79	kJ/mol	Joback Method
hf	-600.97	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.785		Crippen Method
mcvol	262.570	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
tb	817.66	K	Joback Method
tc	1028.55	K	Joback Method
tf	503.21	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.62	J/mol×K	817.66	Joback Method
cpg	723.04	J/mol×K	852.81	Joback Method
cpg	735.46	J/mol×K	887.96	Joback Method
cpg	746.89	J/mol×K	923.11	Joback Method
cpg	757.34	J/mol×K	958.26	Joback Method

cpg	766.83	J/mol×K	993.40	Joback Method
cpg	775.36	J/mol×K	1028.55	Joback Method
dvisc	0.0004920	Pa×s	503.21	Joback Method
dvisc	0.0002944	Pa×s	555.62	Joback Method
dvisc	0.0001925	Pa×s	608.03	Joback Method
dvisc	0.0001347	Pa×s	660.43	Joback Method
dvisc	0.0000993	Pa×s	712.84	Joback Method
dvisc	0.0000763	Pa×s	765.25	Joback Method
dvisc	0.0000607	Pa×s	817.66	Joback Method
hvapt	85.40	kJ/mol	517.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928478&Units=SI
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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