

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/molxK	817.66	Joback Method
cpg	723.04	J/molxK	852.81	Joback Method
cpg	735.46	J/molxK	887.96	Joback Method
cpg	746.89	J/molxK	923.11	Joback Method
cpg	757.34	J/molxK	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	Paxs	503.21	Joback Method
dvisc	0.0002944	Paxs	555.62	Joback Method
dvisc	0.0001925	Paxs	608.03	Joback Method
dvisc	0.0001347	Paxs	660.43	Joback Method
dvisc	0.0000993	Paxs	712.84	Joback Method
dvisc	0.0000763	Paxs	765.25	Joback Method
dvisc	0.0000607	Paxs	817.66	Joback Method
hvapt	85.40	kJ/mol	517.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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