Diethylmalonic acid, 2,2-dichloroethyl heptyl ester

Inchi: InChI=1S/C16H28Cl2O4/c1-4-7-8-9-10-11-21-14(19)16(5-2,6-3)15(20)22-12-13(17)18/h1

InchiKey: PQOKSVSJWIPGKL-UHFFFAOYSA-N

Formula: C16H28Cl2O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 355.30

Physical Properties

Property code	Value	Unit	Source
gf	-407.46	kJ/mol	Joback Method
hf	-908.68	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	76.61	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.653		Crippen Method
mcvol	275.660	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	789.25	K	Joback Method
tc	982.56	K	Joback Method
tf	461.66	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.19	J/mol×K	789.25	Joback Method
cpg	811.26	J/mol×K	821.47	Joback Method
cpg	825.38	J/mol×K	853.69	Joback Method
cpg	838.58	J/mol×K	885.91	Joback Method
cpg	850.89	J/mol×K	918.12	Joback Method
cpg	862.34	J/mol×K	950.34	Joback Method
cpg	872.96	J/mol×K	982.56	Joback Method
dvisc	0.0009059	Pa×s	461.66	Joback Method

dvisc	0.0004378	Pa×s	516.26	Joback Method
dvisc	0.0002431	Pa×s	570.86	Joback Method
dvisc	0.0001496	Pa×s	625.45	Joback Method
dvisc	0.0000995	Pa×s	680.05	Joback Method
dvisc	0.0000704	Pa×s	734.65	Joback Method
dvisc	0.0000522	Pa×s	789.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370782&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
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