Diethylmalonic acid, 2,2-dichloroethyl pentyl ester

Inchi: InChI=1S/C14H24Cl2O4/c1-4-7-8-9-19-12(17)14(5-2,6-3)13(18)20-10-11(15)16/h11H,4-1

InchiKey: AWWOJXTUMZTEPW-UHFFFAOYSA-N

Formula: C14H24Cl2O4

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

Mol. weight [g/mol]: 327.24

Physical Properties

Property code	Value	Unit	Source
gf	-424.30	kJ/mol	Joback Method
hf	-867.40	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.873		Crippen Method
mcvol	247.480	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	1803.00		NIST Webbook
tb	743.49	K	Joback Method
tc	937.53	K	Joback Method
tf	439.12	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.03	J/mol×K	743.49	Joback Method
cpg	747.38	J/mol×K	905.19	Joback Method
cpg	736.38	J/mol×K	872.85	Joback Method
cpg	724.57	J/mol×K	840.51	Joback Method
cpg	711.92	J/mol×K	808.17	Joback Method
cpg	698.42	J/mol×K	775.83	Joback Method
cpg	757.60	J/mol×K	937.53	Joback Method
dvisc	0.0000711	Pa×s	743.49	Joback Method
dvisc	0.0000955	Pa×s	692.76	Joback Method

dvisc	0.0001342	Pa×s	642.03	Joback Method
dvisc	0.0002000	Pa×s	591.31	Joback Method
dvisc	0.0003213	Pa×s	540.58	Joback Method
dvisc	0.0005693	Pa×s	489.85	Joback Method
dvisc	0.0011514	Pa×s	439.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370780&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