Diethylmalonic acid, monochloride, 2-ethylhexyl ester

Inchi: InChI=1S/C15H27ClO3/c1-5-9-10-12(6-2)11-19-14(18)15(7-3,8-4)13(16)17/h12H,5-11H2

InchiKey: ZQXZYIIBTYRPKI-UHFFFAOYSA-N

Formula: C15H27ClO3

SMILES: CCCCC(CC)COC(=O)C(CC)(CC)C(=O)Cl

Mol. weight [g/mol]: 290.83

Physical Properties

Property code	Value	Unit	Source
gf	-298.95	kJ/mol	Joback Method
hf	-740.08	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.318		Crippen Method
mcvol	243.460	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	706.52	K	Joback Method
tc	895.71	K	Joback Method
tf	398.24	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.13	J/mol×K	706.52	Joback Method
cpg	698.19	J/mol×K	738.05	Joback Method
cpg	713.36	J/mol×K	769.58	Joback Method
cpg	727.66	J/mol×K	801.11	Joback Method
cpg	741.13	J/mol×K	832.65	Joback Method
cpg	753.80	J/mol×K	864.18	Joback Method
cpg	765.70	J/mol×K	895.71	Joback Method
dvisc	0.0020173	Pa×s	398.24	Joback Method

dvisc	0.0009067	Pa×s	449.62	Joback Method
dvisc	0.0004802	Pa×s	501.00	Joback Method
dvisc	0.0002862	Pa×s	552.38	Joback Method
dvisc	0.0001863	Pa×s	603.76	Joback Method
dvisc	0.0001297	Pa×s	655.14	Joback Method
dvisc	0.0000952	Pa×s	706.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369633&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
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
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