Diethylmalonic acid, monochloride, decyl ester

Inchi: InChI=1S/C17H31ClO3/c1-4-7-8-9-10-11-12-13-14-21-16(20)17(5-2,6-3)15(18)19/h4-14H

InchiKey: KSWCHIVJMVRMIO-UHFFFAOYSA-N

Formula: C17H31ClO3

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Cl

Mol. weight [g/mol]: 318.88

Physical Properties

Property code	Value	Unit	Source
gf	-279.67	kJ/mol	Joback Method
hf	-776.08	kJ/mol	Joback Method
hfus	40.95	kJ/mol	Joback Method
hvap	72.43	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.242		Crippen Method
mcvol	271.640	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	752.72	K	Joback Method
tc	938.73	K	Joback Method
tf	435.78	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.32	J/mol×K	752.72	Joback Method
cpg	868.16	J/mol×K	907.73	Joback Method
cpg	855.08	J/mol×K	876.73	Joback Method
cpg	841.19	J/mol×K	845.73	Joback Method
cpg	826.46	J/mol×K	814.72	Joback Method
cpg	810.85	J/mol×K	783.72	Joback Method
cpg	880.47	J/mol×K	938.73	Joback Method
dvisc	0.0000768	Pa×s	752.72	Joback Method

dvisc	0.0001032	Pa×s	699.90	Joback Method
dvisc	0.0001453	Pa×s	647.07	Joback Method
dvisc	0.0002176	Pa×s	594.25	Joback Method
dvisc	0.0003524	Pa×s	541.43	Joback Method
dvisc	0.0006336	Pa×s	488.60	Joback Method
dvisc	0.0013130	Pa×s	435.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369507&Units=SI

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