Diethylmalonic acid, monochloride, 1-naphthyl ester

Inchi: InChI=1S/C17H17ClO3/c1-3-17(4-2,15(18)19)16(20)21-14-11-7-9-12-8-5-6-10-13(12)14/

InchiKey: ZMIIMTSBUKCSFR-UHFFFAOYSA-N

Formula: C17H17ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1cccc2ccccc12

Mol. weight [g/mol]: 304.77

Physical Properties

Property code	Value	Unit	Source
gf	-70.24	kJ/mol	Joback Method
hf	-359.95	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.317		Crippen Method
mcvol	228.420	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	803.36	K	Joback Method
tc	1037.55	K	Joback Method
tf	507.42	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.87	J/mol×K	803.36	Joback Method
cpg	646.13	J/mol×K	842.39	Joback Method
cpg	658.37	J/mol×K	881.42	Joback Method
cpg	669.68	J/mol×K	920.45	Joback Method
cpg	680.18	J/mol×K	959.48	Joback Method
cpg	689.94	J/mol×K	998.52	Joback Method
cpg	699.09	J/mol×K	1037.55	Joback Method
dvisc	0.0009859	Pa×s	507.42	Joback Method
dvisc	0.0006238	Pa×s	556.74	Joback Method

dvisc	0.0004252	Pa×s	606.07	Joback Method
dvisc	0.0003070	Pa×s	655.39	Joback Method
dvisc	0.0002320	Pa×s	704.71	Joback Method
dvisc	0.0001819	Pa×s	754.04	Joback Method
dvisc	0.0001469	Pa×s	803.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369877&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