Diethylmalonic acid, monochloride, nonyl ester

Inchi: InChI=1S/C16H29ClO3/c1-4-7-8-9-10-11-12-13-20-15(19)16(5-2,6-3)14(17)18/h4-13H2,1

InchiKey: JKSJCDXKBDRPRY-UHFFFAOYSA-N

Formula: C16H29ClO3

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

Mol. weight [g/mol]: 304.85

Physical Properties

Property code	Value	Unit	Source
gf	-288.09	kJ/mol	Joback Method
hf	-755.44	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.852		Crippen Method
mcvol	257.550	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	1577.00		NIST Webbook
tb	729.84	K	Joback Method
tc	915.88	K	Joback Method
tf	424.51	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.43	J/mol×K	729.84	Joback Method
cpg	753.62	J/mol×K	760.85	Joback Method
cpg	768.91	J/mol×K	791.85	Joback Method
cpg	783.35	J/mol×K	822.86	Joback Method
cpg	796.97	J/mol×K	853.87	Joback Method
cpg	809.79	J/mol×K	884.88	Joback Method
cpg	821.86	J/mol×K	915.88	Joback Method
dvisc	0.0014674	Pa×s	424.51	Joback Method
dvisc	0.0007164	Pa×s	475.40	Joback Method

dvisc	0.0004018	Pa×s	526.29	Joback Method
dvisc	0.0002495	Pa×s	577.17	Joback Method
dvisc	0.0001674	Pa×s	628.06	Joback Method
dvisc	0.0001192	Pa×s	678.95	Joback Method
dvisc	0.0000890	Pa×s	729.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369472&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