Diethylmalonic acid, monochloride, dodecyl ester

Inchi: InChI=1S/C19H35ClO3/c1-4-7-8-9-10-11-12-13-14-15-16-23-18(22)19(5-2,6-3)17(20)21/

InchiKey: IXMLNPATLHEMKN-UHFFFAOYSA-N

Formula: C19H35ClO3

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

Mol. weight [g/mol]: 346.93

Physical Properties

Property code	Value	Unit	Source
gf	-262.83	kJ/mol	Joback Method
hf	-817.36	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	76.88	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	6.022		Crippen Method
mcvol	299.820	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	798.48	K	Joback Method
tc	986.18	K	Joback Method
tf	458.32	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.03	J/mol×K	798.48	Joback Method
cpg	928.24	J/mol×K	829.76	Joback Method
cpg	944.47	J/mol×K	861.05	Joback Method
cpg	959.77	J/mol×K	892.33	Joback Method
cpg	974.17	J/mol×K	923.62	Joback Method
cpg	987.72	J/mol×K	954.90	Joback Method
cpg	1000.46	J/mol×K	986.18	Joback Method
dvisc	0.0010388	Pa×s	458.32	Joback Method

dvisc	0.0004903	Pa×s	515.01	Joback Method
dvisc	0.0002686	Pa×s	571.71	Joback Method
dvisc	0.0001640	Pa×s	628.40	Joback Method
dvisc	0.0001087	Pa×s	685.09	Joback Method
dvisc	0.0000767	Pa×s	741.79	Joback Method
dvisc	0.0000568	Pa×s	798.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369722&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