Diethylmalonic acid, monochloride, 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C15H27ClO3/c1-7-15(8-2,12(16)17)13(18)19-10-11(3)9-14(4,5)6/h11H,7-10H2

InchiKey: BFCBLBSMZGPTHY-UHFFFAOYSA-N

Formula: C15H27ClO3

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

Mol. weight [g/mol]: 290.83

Physical Properties

Property code	Value	Unit	Source
gf	-296.11	kJ/mol	Joback Method
hf	-748.83	kJ/mol	Joback Method
hfus	24.84	kJ/mol	Joback Method
hvap	66.29	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.174		Crippen Method
mcvol	243.460	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	1583.00		NIST Webbook
tb	703.29	K	Joback Method
tc	900.49	K	Joback Method
tf	400.66	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.49	J/mol×K	703.29	Joback Method
cpg	757.48	J/mol×K	867.62	Joback Method
cpg	744.68	J/mol×K	834.76	Joback Method
cpg	731.04	J/mol×K	801.89	Joback Method
cpg	716.50	J/mol×K	769.02	Joback Method
cpg	701.00	J/mol×K	736.16	Joback Method
cpg	769.47	J/mol×K	900.49	Joback Method
dvisc	0.0000800	Pa×s	703.29	Joback Method
dvisc	0.0001116	Pa×s	652.85	Joback Method

dvisc	0.0001645	Pa×s	602.41	Joback Method
dvisc	0.0002604	Pa×s	551.97	Joback Method
dvisc	0.0004520	Pa×s	501.54	Joback Method
dvisc	0.0008878	Pa×s	451.10	Joback Method
dvisc	0.0020665	Pa×s	400.66	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=U369492&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