

Diethylmalonic acid, monochloride, hexyl ester

Inchi:	InChI=1S/C13H23ClO3/c1-4-7-8-9-10-17-12(16)13(5-2,6-3)11(14)15/h4-10H2,1-3H3
InchiKey:	ZXXOWJUQLRKQDM-UHFFFAOYSA-N
Formula:	C13H23ClO3
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	262.77

Physical Properties

Property code	Value	Unit	Source
gf	-313.35	kJ/mol	Joback Method
hf	-693.52	kJ/mol	Joback Method
hfus	30.59	kJ/mol	Joback Method
hvap	63.52	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.682		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinsol	1541.00		NIST Webbook
tb	661.20	K	Joback Method
tc	850.26	K	Joback Method
tf	390.70	K	Joback Method
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.58	J/molxK	661.20	Joback Method
cpg	640.68	J/molxK	818.75	Joback Method
cpg	628.78	J/molxK	787.24	Joback Method
cpg	616.15	J/molxK	755.73	Joback Method
cpg	602.76	J/molxK	724.22	Joback Method
cpg	588.58	J/molxK	692.71	Joback Method
cpg	651.87	J/molxK	850.26	Joback Method
dvisc	0.0001363	Paxs	661.20	Joback Method
dvisc	0.0001810	Paxs	616.12	Joback Method

dvisc	0.0002512	Paxs	571.03	Joback Method
dvisc	0.0003690	Paxs	525.95	Joback Method
dvisc	0.0005825	Paxs	480.87	Joback Method
dvisc	0.0010105	Paxs	435.78	Joback Method
dvisc	0.0019909	Paxs	390.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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