

Diethylmalonic acid, monochloride, hept-4-yl ester

Inchi:	InChI=1S/C14H25ClO3/c1-5-9-11(10-6-2)18-13(17)14(7-3,8-4)12(15)16/h11H,5-10H2,1-
InchiKey:	KCGIYFVESAUEMY-UHFFFAOYSA-N
Formula:	C14H25ClO3
SMILES:	CCCC(CCC)OC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	276.80

Physical Properties

Property code	Value	Unit	Source
gf	-307.37	kJ/mol	Joback Method
hf	-719.44	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.070		Crippen Method
mcvol	229.370	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1526.00		NIST Webbook
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tb	683.64	K	Joback Method
tc	874.11	K	Joback Method
tf	386.97	K	Joback Method
vc	0.881	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.47	J/molxK	683.64	Joback Method
cpg	697.49	J/molxK	842.36	Joback Method
cpg	685.12	J/molxK	810.62	Joback Method
cpg	671.96	J/molxK	778.87	Joback Method
cpg	657.99	J/molxK	747.13	Joback Method
cpg	643.17	J/molxK	715.38	Joback Method
cpg	709.11	J/molxK	874.11	Joback Method
dvisc	0.0001099	Paxs	683.64	Joback Method

dvisc	0.0001494	Paxs	634.19	Joback Method
dvisc	0.0002140	Paxs	584.75	Joback Method
dvisc	0.0003274	Paxs	535.31	Joback Method
dvisc	0.0005463	Paxs	485.86	Joback Method
dvisc	0.0010237	Paxs	436.42	Joback Method
dvisc	0.0022520	Paxs	386.97	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370522&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

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