

Diethylmalonic acid, monochloride, heptyl ester

Inchi:	InChI=1S/C14H25ClO3/c1-4-7-8-9-10-11-18-13(17)14(5-2,6-3)12(15)16/h4-11H2,1-3H3
InchiKey:	RIHXWQJYBRAOMP-UHFFFAOYSA-N
Formula:	C14H25ClO3
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	276.80

Physical Properties

Property code	Value	Unit	Source
gf	-304.93	kJ/mol	Joback Method
hf	-714.16	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.072		Crippen Method
mvol	229.370	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	684.08	K	Joback Method
tc	871.70	K	Joback Method
tf	401.97	K	Joback Method
vc	0.887	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.98	J/molxK	684.08	Joback Method
cpg	642.42	J/molxK	715.35	Joback Method
cpg	657.01	J/molxK	746.62	Joback Method
cpg	670.79	J/molxK	777.89	Joback Method
cpg	683.78	J/molxK	809.16	Joback Method
cpg	696.02	J/molxK	840.43	Joback Method
cpg	707.54	J/molxK	871.70	Joback Method
dvisc	0.0018077	Paxs	401.97	Joback Method

dvisc	0.0009052	Paxs	448.99	Joback Method
dvisc	0.0005168	Paxs	496.01	Joback Method
dvisc	0.0003251	Paxs	543.02	Joback Method
dvisc	0.0002202	Paxs	590.04	Joback Method
dvisc	0.0001580	Paxs	637.06	Joback Method
dvisc	0.0001186	Paxs	684.08	Joback Method

Sources

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=U369527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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