

Malonic acid, 2,2-dichloroethyl heptyl ester

Inchi:	InChI=1S/C12H20Cl2O4/c1-2-3-4-5-6-7-17-11(15)8-12(16)18-9-10(13)14/h10H,2-9H2,1H
InchiKey:	UPSFVOVWXAXHHD-UHFFFAOYSA-N
Formula:	C12H20Cl2O4
SMILES:	CCCCCCCOC(=O)CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	299.19

Physical Properties

Property code	Value	Unit	Source
gf	-443.98	kJ/mol	Joback Method
hf	-817.37	kJ/mol	Joback Method
hfus	37.28	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.237		Crippen Method
mvol	219.300	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	700.96	K	Joback Method
tc	889.73	K	Joback Method
tf	414.16	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.54	J/molxK	700.96	Joback Method
cpg	586.79	J/molxK	732.42	Joback Method
cpg	599.31	J/molxK	763.88	Joback Method
cpg	611.11	J/molxK	795.34	Joback Method
cpg	622.19	J/molxK	826.80	Joback Method
cpg	632.56	J/molxK	858.26	Joback Method
cpg	642.22	J/molxK	889.73	Joback Method
dvisc	0.0014300	Paxs	414.16	Joback Method
dvisc	0.0007549	Paxs	461.96	Joback Method

dvisc	0.0004492	Paxs	509.76	Joback Method
dvisc	0.0002922	Paxs	557.56	Joback Method
dvisc	0.0002034	Paxs	605.36	Joback Method
dvisc	0.0001493	Paxs	653.16	Joback Method
dvisc	0.0001143	Paxs	700.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349062&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
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

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