

Malonic acid, 8-chlorooctyl ethyl ester

Inchi:	InChI=1S/C13H23ClO4/c1-2-17-12(15)11-13(16)18-10-8-6-4-3-5-7-9-14/h2-11H2,1H3
InchiKey:	QVPHPCBYJIWUMA-UHFFFAOYSA-N
Formula:	C13H23ClO4
SMILES:	CCOC(=O)CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	278.77

Physical Properties

Property code	Value	Unit	Source
gf	-421.19	kJ/mol	Joback Method
hf	-816.99	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.062		Crippen Method
mvol	221.150	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	686.85	K	Joback Method
tc	867.86	K	Joback Method
tf	410.51	K	Joback Method
vc	0.861	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.34	J/molxK	686.85	Joback Method
cpg	612.70	J/molxK	717.02	Joback Method
cpg	626.35	J/molxK	747.19	Joback Method
cpg	639.30	J/molxK	777.35	Joback Method
cpg	651.53	J/molxK	807.52	Joback Method
cpg	663.07	J/molxK	837.69	Joback Method
cpg	673.92	J/molxK	867.86	Joback Method
dvisc	0.0013375	Paxs	410.51	Joback Method

dvisc	0.0007339	Paxs	456.57	Joback Method
dvisc	0.0004495	Paxs	502.62	Joback Method
dvisc	0.0002990	Paxs	548.68	Joback Method
dvisc	0.0002118	Paxs	594.74	Joback Method
dvisc	0.0001577	Paxs	640.79	Joback Method
dvisc	0.0001221	Paxs	686.85	Joback Method

Sources

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=U349002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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