

Malonic acid, 8-chlorooctyl isobutyl ester

Inchi:	InChI=1S/C15H27ClO4/c1-13(2)12-20-15(18)11-14(17)19-10-8-6-4-3-5-7-9-16/h13H,3-1
InchiKey:	HSJUCFNMXKNWJC-UHFFFAOYSA-N
Formula:	C15H27ClO4
SMILES:	CC(C)COC(=O)CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	306.82

Physical Properties

Property code	Value	Unit	Source
gf	-406.79	kJ/mol	Joback Method
hf	-863.55	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.698		Crippen Method
mcvol	249.330	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinqol	2079.00		NIST Webbook
tb	732.17	K	Joback Method
tc	914.96	K	Joback Method
tf	418.05	K	Joback Method
vc	0.967	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.70	J/molxK	732.17	Joback Method
cpg	724.18	J/molxK	762.64	Joback Method
cpg	738.83	J/molxK	793.10	Joback Method
cpg	752.66	J/molxK	823.57	Joback Method
cpg	765.68	J/molxK	854.03	Joback Method
cpg	777.89	J/molxK	884.50	Joback Method
cpg	789.31	J/molxK	914.96	Joback Method
dvisc	0.0013342	Paxs	418.05	Joback Method
dvisc	0.0006557	Paxs	470.40	Joback Method

dvisc	0.0003715	Paxs	522.76	Joback Method
dvisc	0.0002334	Paxs	575.11	Joback Method
dvisc	0.0001585	Paxs	627.46	Joback Method
dvisc	0.0001142	Paxs	679.82	Joback Method
dvisc	0.0000863	Paxs	732.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349004&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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