

Malonic acid, butyl 8-chlorooctyl ester

Inchi:	InChI=1S/C15H27ClO4/c1-2-3-11-19-14(17)13-15(18)20-12-9-7-5-4-6-8-10-16/h2-13H2,
InchiKey:	BPVJFODNWKIIMW-UHFFFAOYSA-N
Formula:	C15H27ClO4
SMILES:	CCCCOC(=O)CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	306.82

Physical Properties

Property code	Value	Unit	Source
gf	-404.35	kJ/mol	Joback Method
hf	-858.27	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.842		Crippen Method
mvol	249.330	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2118.00		NIST Webbook
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tb	732.61	K	Joback Method
tc	913.43	K	Joback Method
tf	433.05	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.19	J/molxK	732.61	Joback Method
cpg	723.48	J/molxK	762.75	Joback Method
cpg	737.98	J/molxK	792.88	Joback Method
cpg	751.68	J/molxK	823.02	Joback Method
cpg	764.59	J/molxK	853.16	Joback Method
cpg	776.72	J/molxK	883.29	Joback Method
cpg	788.08	J/molxK	913.43	Joback Method
dvisc	0.0011207	Paxs	433.05	Joback Method

dvisc	0.0005981	Paxs	482.98	Joback Method
dvisc	0.0003590	Paxs	532.90	Joback Method
dvisc	0.0002352	Paxs	582.83	Joback Method
dvisc	0.0001647	Paxs	632.76	Joback Method
dvisc	0.0001215	Paxs	682.68	Joback Method
dvisc	0.0000935	Paxs	732.61	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=U349005&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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