

Malonic acid, 8-chlorooctyl propyl ester

Inchi:	InChI=1S/C14H25ClO4/c1-2-10-18-13(16)12-14(17)19-11-8-6-4-3-5-7-9-15/h2-12H2,1H3
InchiKey:	CSXNAOIJZYGGFP-UHFFFAOYSA-N
Formula:	C14H25ClO4
SMILES:	CCCOC(=O)CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	292.80

Physical Properties

Property code	Value	Unit	Source
gf	-412.77	kJ/mol	Joback Method
hf	-837.63	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.452		Crippen Method
mcvol	235.240	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpola	2026.00		NIST Webbook
tb	709.73	K	Joback Method
tc	890.40	K	Joback Method
tf	421.78	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.67	J/molxK	709.73	Joback Method
cpg	667.51	J/molxK	739.84	Joback Method
cpg	681.60	J/molxK	769.95	Joback Method
cpg	694.94	J/molxK	800.06	Joback Method
cpg	707.54	J/molxK	830.17	Joback Method
cpg	719.39	J/molxK	860.29	Joback Method
cpg	730.52	J/molxK	890.40	Joback Method
dvisc	0.0012278	Paxs	421.78	Joback Method
dvisc	0.0006642	Paxs	469.77	Joback Method

dvisc	0.0004027	Paxs	517.76	Joback Method
dvisc	0.0002657	Paxs	565.75	Joback Method
dvisc	0.0001872	Paxs	613.75	Joback Method
dvisc	0.0001387	Paxs	661.74	Joback Method
dvisc	0.0001070	Paxs	709.73	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=U349003&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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