

Malonic acid, 10-chlorodecyl propyl ester

Inchi:	InChI=1S/C16H29ClO4/c1-2-12-20-15(18)14-16(19)21-13-10-8-6-4-3-5-7-9-11-17/h2-14H
InchiKey:	COEZQPUULVJOAL-UHFFFAOYSA-N
Formula:	C16H29ClO4
SMILES:	CCCOC(=O)CC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]:	320.85

Physical Properties

Property code	Value	Unit	Source
gf	-395.93	kJ/mol	Joback Method
hf	-878.91	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.232		Crippen Method
mvol	263.420	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	755.49	K	Joback Method
tc	937.01	K	Joback Method
tf	444.32	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.82	J/molxK	755.49	Joback Method
cpg	835.01	J/molxK	906.75	Joback Method
cpg	822.63	J/molxK	876.50	Joback Method
cpg	809.43	J/molxK	846.25	Joback Method
cpg	795.41	J/molxK	816.00	Joback Method
cpg	780.54	J/molxK	785.74	Joback Method
cpg	846.57	J/molxK	937.01	Joback Method
dvisc	0.0000814	Paxs	755.49	Joback Method

dvisc	0.0001062	Paxs	703.63	Joback Method
dvisc	0.0001445	Paxs	651.77	Joback Method
dvisc	0.0002074	Paxs	599.90	Joback Method
dvisc	0.0003188	Paxs	548.04	Joback Method
dvisc	0.0005360	Paxs	496.18	Joback Method
dvisc	0.0010176	Paxs	444.32	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=U349039&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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