

Dimethylmalonic acid, monochloride, decyl ester

Inchi:	InChI=1S/C15H27ClO3/c1-4-5-6-7-8-9-10-11-12-19-14(18)15(2,3)13(16)17/h4-12H2,1-3H1
InchiKey:	PEQBNQPKXJIGOR-UHFFFAOYSA-N
Formula:	C15H27ClO3
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	290.83

Physical Properties

Property code	Value	Unit	Source
gf	-296.51	kJ/mol	Joback Method
hf	-734.80	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.462		Crippen Method
mcvol	243.460	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinsol	1817.00		NIST Webbook
tb	706.96	K	Joback Method
tc	893.56	K	Joback Method
tf	413.24	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.63	J/molxK	706.96	Joback Method
cpg	697.45	J/molxK	738.06	Joback Method
cpg	712.41	J/molxK	769.16	Joback Method
cpg	726.54	J/molxK	800.26	Joback Method
cpg	739.86	J/molxK	831.36	Joback Method
cpg	752.40	J/molxK	862.46	Joback Method
cpg	764.21	J/molxK	893.56	Joback Method
dvisc	0.0016327	Paxs	413.24	Joback Method
dvisc	0.0008070	Paxs	462.19	Joback Method

dvisc	0.0004565	Paxs	511.15	Joback Method
dvisc	0.0002853	Paxs	560.10	Joback Method
dvisc	0.0001923	Paxs	609.05	Joback Method
dvisc	0.0001375	Paxs	658.01	Joback Method
dvisc	0.0001029	Paxs	706.96	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=U361714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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