

Diethylmalonic acid, monochloride, 2-octyl ester

Inchi:	InChI=1S/C15H27ClO3/c1-5-8-9-10-11-12(4)19-14(18)15(6-2,7-3)13(16)17/h12H,5-11H2
InchiKey:	UJURCJPVEKCCCH-UHFFFAOYSA-N
Formula:	C15H27ClO3
SMILES:	CCCCCCC(C)OC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	290.83

Physical Properties

Property code	Value	Unit	Source
gf	-298.95	kJ/mol	Joback Method
hf	-740.08	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.460		Crippen Method
mvol	243.460	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	706.52	K	Joback Method
tc	895.71	K	Joback Method
tf	398.24	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.13	J/molxK	706.52	Joback Method
cpg	698.19	J/molxK	738.05	Joback Method
cpg	713.36	J/molxK	769.58	Joback Method
cpg	727.66	J/molxK	801.11	Joback Method
cpg	741.13	J/molxK	832.65	Joback Method
cpg	753.80	J/molxK	864.18	Joback Method
cpg	765.70	J/molxK	895.71	Joback Method
dvisc	0.0020173	Paxs	398.24	Joback Method
dvisc	0.0009067	Paxs	449.62	Joback Method

dvisc	0.0004802	Paxs	501.00	Joback Method
dvisc	0.0002862	Paxs	552.38	Joback Method
dvisc	0.0001863	Paxs	603.76	Joback Method
dvisc	0.0001297	Paxs	655.14	Joback Method
dvisc	0.0000952	Paxs	706.52	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=U369380&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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