

Dimethylmalonic acid, monochloride, heptyl ester

Inchi:	InChI=1S/C12H21ClO3/c1-4-5-6-7-8-9-16-11(15)12(2,3)10(13)14/h4-9H2,1-3H3
InchiKey:	GVVJLYXWQBWNLX-UHFFFAOYSA-N
Formula:	C12H21ClO3
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	248.75

Physical Properties

Property code	Value	Unit	Source
gf	-321.77	kJ/mol	Joback Method
hf	-672.88	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.292		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	638.32	K	Joback Method
tc	829.20	K	Joback Method
tf	379.43	K	Joback Method
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.50	J/mol×K	638.32	Joback Method
cpg	536.01	J/mol×K	670.13	Joback Method
cpg	549.73	J/mol×K	701.95	Joback Method
cpg	562.69	J/mol×K	733.76	Joback Method
cpg	574.90	J/mol×K	765.57	Joback Method
cpg	586.40	J/mol×K	797.39	Joback Method
cpg	597.22	J/mol×K	829.20	Joback Method
dvisc	0.0021798	Paxs	379.43	Joback Method
dvisc	0.0011224	Paxs	422.58	Joback Method

dvisc	0.0006535	Paxs	465.73	Joback Method
dvisc	0.0004171	Paxs	508.88	Joback Method
dvisc	0.0002855	Paxs	552.02	Joback Method
dvisc	0.0002065	Paxs	595.17	Joback Method
dvisc	0.0001561	Paxs	638.32	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=U361910&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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