

Dimethylmalonic acid, heptyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C18H23Cl3O4/c1-4-5-6-7-8-9-24-16(22)18(2,3)17(23)25-15-13(20)10-12(19)1
InchiKey:	WIIPCGXAPJBWFA-UHFFFAOYSA-N
Formula:	C18H23Cl3O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	409.73

Physical Properties

Property code	Value	Unit	Source
gf	-316.59	kJ/mol	Joback Method
hf	-758.30	kJ/mol	Joback Method
hfus	46.00	kJ/mol	Joback Method
hvap	90.09	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.092		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	2459.00		NIST Webbook
tb	914.50	K	Joback Method
tc	1135.04	K	Joback Method
tf	593.10	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.05	J/molxK	914.50	Joback Method
cpg	847.20	J/molxK	951.26	Joback Method
cpg	858.26	J/molxK	988.01	Joback Method
cpg	868.27	J/molxK	1024.77	Joback Method
cpg	877.26	J/molxK	1061.53	Joback Method
cpg	885.29	J/molxK	1098.28	Joback Method
cpg	892.37	J/molxK	1135.04	Joback Method
dvisc	0.0002724	Paxs	593.10	Joback Method
dvisc	0.0001700	Paxs	646.67	Joback Method

dvisc	0.0001140	Paxs	700.23	Joback Method
dvisc	0.0000809	Paxs	753.80	Joback Method
dvisc	0.0000601	Paxs	807.37	Joback Method
dvisc	0.0000464	Paxs	860.93	Joback Method
dvisc	0.0000368	Paxs	914.50	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=U363651&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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