Dimethylmalonic acid, heptyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C18H23Cl3O4/c1-4-5-6-7-8-9-24-16(22)18(2,3)17(23)25-14-11-12(19)10-13(20

InchiKey: UBQBCCNUVRRNBT-UHFFFAOYSA-N

Formula: C18H23Cl3O4

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl

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	2521.00		NIST Webbook
rinpol	2521.00		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/mol×K	914.50	Joback Method
cpg	847.20	J/mol×K	951.26	Joback Method
cpg	858.26	J/mol×K	988.01	Joback Method
cpg	868.27	J/mol×K	1024.77	Joback Method
cpg	877.26	J/mol×K	1061.53	Joback Method
cpg	885.29	J/mol×K	1098.28	Joback Method
cpg	892.37	J/mol×K	1135.04	Joback Method
dvisc	0.0002724	Pa×s	593.10	Joback Method

dvisc	0.0001700	Pa×s	646.67	Joback Method
dvisc	0.0001140	Pa×s	700.23	Joback Method
dvisc	0.0000809	Pa×s	753.80	Joback Method
dvisc	0.0000601	Pa×s	807.37	Joback Method
dvisc	0.0000464	Pa×s	860.93	Joback Method
dvisc	0.0000368	Pa×s	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=U363909&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