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

Inchi: InChI=1S/C28H43Cl3O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-34-26(32)28(2,3

InchiKey: YJAVNYKDKBGGRS-UHFFFAOYSA-N

Formula: C28H43Cl3O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 550.00

Physical Properties

Property code	Value	Unit	Source
gf	-232.39	kJ/mol	Joback Method
hf	-964.70	kJ/mol	Joback Method
hfus	71.90	kJ/mol	Joback Method
hvap	112.35	kJ/mol	Joback Method
log10ws	-10.83		Crippen Method
logp	9.993		Crippen Method
mcvol	433.220	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinpol	3500.00		NIST Webbook
tb	1143.30	K	Joback Method
tc	1411.80	K	Joback Method
tf	705.80	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.64	J/mol×K	1143.30	Joback Method
cpg	1452.28	J/mol×K	1188.05	Joback Method
cpg	1465.18	J/mol×K	1232.80	Joback Method
cpg	1476.48	J/mol×K	1277.55	Joback Method
cpg	1486.31	J/mol×K	1322.30	Joback Method
cpg	1494.80	J/mol×K	1367.05	Joback Method
cpg	1502.07	J/mol×K	1411.80	Joback Method
dvisc	0.0000765	Pa×s	705.80	Joback Method
dvisc	0.0000431	Pa×s	778.72	Joback Method

dvisc	0.0000268	Pa×s	851.63	Joback Method
dvisc	0.0000180	Pa×s	924.55	Joback Method
dvisc	0.0000128	Pa×s	997.47	Joback Method
dvisc	0.0000095	Pa×s	1070.38	Joback Method
dvisc	0.0000074	Pa×s	1143.30	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=U363659&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