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

Inchi: InChI=1S/C21H29Cl3O4/c1-4-5-6-7-8-9-10-11-12-27-19(25)21(2,3)20(26)28-17-14-15(22
InchiKey: BPYNSAWLBYJABD-UHFFFAOYSA-N
Formula: C21H29Cl3O4
SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	-291.33	kJ/mol	Joback Method
hf	-820.22	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	96.77	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.262		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	983.14	K	Joback Method
tc	1207.14	K	Joback Method
tf	626.91	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.50	J/mol×K	983.14	Joback Method
cpg	1023.25	J/mol×K	1020.47	Joback Method
cpg	1034.79	J/mol×K	1057.81	Joback Method
cpg	1045.18	J/mol×K	1095.14	Joback Method
cpg	1054.48	J/mol×K	1132.48	Joback Method
cpg	1062.73	J/mol×K	1169.81	Joback Method
cpg	1069.97	J/mol×K	1207.14	Joback Method
dvisc	0.0001909	Pa×s	626.91	Joback Method

dvisc	0.0001152	Pa×s	686.28	Joback Method
dvisc	0.0000754	Pa×s	745.65	Joback Method
dvisc	0.0000525	Pa×s	805.02	Joback Method
dvisc	0.0000384	Pa×s	864.40	Joback Method
dvisc	0.0000293	Pa×s	923.77	Joback Method
dvisc	0.0000230	Pa×s	983.14	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=U363910&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