Diethylmalonic acid, propyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H19Cl3O4/c1-4-7-22-14(20)16(5-2,6-3)15(21)23-13-9-11(18)10(17)8-12(13

InchiKey: PHWZMIDIGKVDDB-UHFFFAOYSA-N

Formula: C16H19Cl3O4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 381.68

Physical Properties

Property code	Value	Unit	Source
gf	-333.43	kJ/mol	Joback Method
hf	-717.02	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.312		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2270.00		NIST Webbook
tb	868.74	K	Joback Method
tc	1090.97	K	Joback Method
tf	570.56	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.62	J/mol×K	868.74	Joback Method
cpg	733.30	J/mol×K	905.78	Joback Method
cpg	743.96	J/mol×K	942.82	Joback Method
cpg	753.61	J/mol×K	979.86	Joback Method
cpg	762.30	J/mol×K	1016.89	Joback Method
cpg	770.05	J/mol×K	1053.93	Joback Method
cpg	776.89	J/mol×K	1090.97	Joback Method
dvisc	0.0003400	Pa×s	570.56	Joback Method
dvisc	0.0002173	Pa×s	620.26	Joback Method

dvisc	0.0001484	Pa×s	669.95	Joback Method
dvisc	0.0001069	Pa×s	719.65	Joback Method
dvisc	0.0000803	Pa×s	769.35	Joback Method
dvisc	0.0000624	Pa×s	819.04	Joback Method
dvisc	0.0000500	Pa×s	868.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U370529&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