Dimethylmalonic acid, 2,5-dichlorophenyl pentyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-4-5-6-9-21-14(19)16(2,3)15(20)22-13-10-11(17)7-8-12(13)18

InchiKey: RUJZONXDTOMDNX-UHFFFAOYSA-N

Formula: C16H20Cl2O4

SMILES: CCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-311.87	kJ/mol	Joback Method
hf	-689.81	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.658		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2125.00		NIST Webbook
tb	826.33	K	Joback Method
tc	1044.31	K	Joback Method
tf	528.12	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.42	J/mol×K	826.33	Joback Method
cpg	755.12	J/mol×K	1007.98	Joback Method
cpg	746.13	J/mol×K	971.65	Joback Method
cpg	736.19	J/mol×K	935.32	Joback Method
cpg	725.29	J/mol×K	898.99	Joback Method
cpg	713.37	J/mol×K	862.66	Joback Method
cpg	763.21	J/mol×K	1044.31	Joback Method
dvisc	0.0000580	Pa×s	826.33	Joback Method
dvisc	0.0000735	Pa×s	776.63	Joback Method

dvisc	0.0000963	Pa×s	726.93	Joback Method
dvisc	0.0001313	Pa×s	677.22	Joback Method
dvisc	0.0001879	Pa×s	627.52	Joback Method
dvisc	0.0002861	Pa×s	577.82	Joback Method
dvisc	0.0004716	Pa×s	528.12	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=U363681&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