Diethylmalonic acid, heptyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C20H27Cl3O4/c1-4-7-8-9-10-11-26-18(24)20(5-2,6-3)19(25)27-17-15(22)12-14

InchiKey: COWVAWHWMVYIQN-UHFFFAOYSA-N

Formula: C20H27Cl3O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 437.79

Physical Properties

Property code	Value	Unit	Source
gf	-299.75	kJ/mol	Joback Method
hf	-799.58	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	94.55	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.872		Crippen Method
mcvol	320.500	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2649.00		NIST Webbook
tb	960.26	K	Joback Method
tc	1182.24	K	Joback Method
tf	615.64	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.39	J/mol×K	960.26	Joback Method
cpg	963.93	J/mol×K	997.26	Joback Method
cpg	975.32	J/mol×K	1034.25	Joback Method
cpg	985.60	J/mol×K	1071.25	Joback Method
cpg	994.81	J/mol×K	1108.25	Joback Method
cpg	1003.00	J/mol×K	1145.24	Joback Method
cpg	1010.21	J/mol×K	1182.24	Joback Method
dvisc	0.0002155	Pa×s	615.64	Joback Method
dvisc	0.0001315	Pa×s	673.08	Joback Method

dvisc	0.0000867	Pa×s	730.51	Joback Method
dvisc	0.0000608	Pa×s	787.95	Joback Method
dvisc	0.0000447	Pa×s	845.39	Joback Method
dvisc	0.0000342	Pa×s	902.82	Joback Method
dvisc	0.0000270	Pa×s	960.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370151&Units=SI
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

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

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