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

Inchi: InChI=1S/C19H25Cl3O4/c1-4-7-8-9-10-25-17(23)19(5-2,6-3)18(24)26-16-12-14(21)13(20

InchiKey: HFAAYHDNMOGJOQ-UHFFFAOYSA-N

Formula: C19H25Cl3O4

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

Mol. weight [g/mol]: 423.76

Physical Properties

Property code	Value	Unit	Source
gf	-308.17	kJ/mol	Joback Method
hf	-778.94	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.482		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	2543.00		NIST Webbook
rinpol	2543.00		NIST Webbook
tb	937.38	K	Joback Method
tc	1158.23	K	Joback Method
tf	604.37	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.89	J/mol×K	937.38	Joback Method
cpg	943.85	J/mol×K	1121.42	Joback Method
cpg	935.73	J/mol×K	1084.61	Joback Method
cpg	926.62	J/mol×K	1047.80	Joback Method
cpg	916.47	J/mol×K	1011.00	Joback Method
cpg	905.24	J/mol×K	974.19	Joback Method
cpg	951.01	J/mol×K	1158.23	Joback Method
dvisc	0.0000316	Pa×s	937.38	Joback Method

dvisc	0.0000398	Pa×s	881.88	Joback Method
dvisc	0.0000519	Pa×s	826.38	Joback Method
dvisc	0.0000702	Pa×s	770.88	Joback Method
dvisc	0.0000995	Pa×s	715.37	Joback Method
dvisc	0.0001497	Pa×s	659.87	Joback Method
dvisc	0.0002426	Pa×s	604.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370533&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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