

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.89	J/molxK	937.38	Joback Method
cpg	905.24	J/molxK	974.19	Joback Method
cpg	916.47	J/molxK	1011.00	Joback Method
cpg	926.62	J/molxK	1047.80	Joback Method
cpg	935.73	J/molxK	1084.61	Joback Method
cpg	943.85	J/molxK	1121.42	Joback Method
cpg	951.01	J/molxK	1158.23	Joback Method
dvisc	0.0002426	Paxs	604.37	Joback Method

dvisc	0.0001497	Paxs	659.87	Joback Method
dvisc	0.0000995	Paxs	715.37	Joback Method
dvisc	0.0000702	Paxs	770.88	Joback Method
dvisc	0.0000519	Paxs	826.38	Joback Method
dvisc	0.0000398	Paxs	881.88	Joback Method
dvisc	0.0000316	Paxs	937.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U370533&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

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