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

Inchi: InChI=1S/C22H31Cl3O4/c1-2-3-4-11-14-28-21(26)12-9-7-5-6-8-10-13-22(27)29-20-16-18
InchiKey: SNSABHPJOFFCCT-UHFFFAOYSA-N
Formula: C22H31Cl3O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 465.84

Physical Properties

Property code	Value	Unit	Source
gf	-285.75	kJ/mol	Joback Method
hf	-832.11	kJ/mol	Joback Method
hfus	63.77	kJ/mol	Joback Method
hvap	100.29	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.796		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	1009.25	K	Joback Method
tc	1235.70	K	Joback Method
tf	635.76	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.88	J/mol×K	1009.25	Joback Method
cpg	1082.67	J/mol×K	1046.99	Joback Method
cpg	1094.07	J/mol×K	1084.73	Joback Method
cpg	1104.10	J/mol×K	1122.48	Joback Method
cpg	1112.81	J/mol×K	1160.22	Joback Method
cpg	1120.23	J/mol×K	1197.96	Joback Method
cpg	1126.38	J/mol×K	1235.70	Joback Method
dvisc	0.0002015	Pa×s	635.76	Joback Method

dvisc	0.0001231	Pa×s	698.01	Joback Method
dvisc	0.0000815	Pa×s	760.26	Joback Method
dvisc	0.0000575	Pa×s	822.50	Joback Method
dvisc	0.0000426	Pa×s	884.75	Joback Method
dvisc	0.0000328	Pa×s	947.00	Joback Method
dvisc	0.0000261	Pa×s	1009.25	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=U355196&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

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