

Sebacic acid, pentyl 2,4,6-trichlorobenzyl ester

Inchi: InChI=1S/C22H31Cl3O4/c1-2-3-10-13-28-21(26)11-8-6-4-5-7-9-12-22(27)29-16-18-19(24)
InchiKey: VXMFSRPGWGRMTG-UHFFFAOYSA-N
Formula: C22H31Cl3O4
SMILES: CCCCCOC(=O)CCCCCCCC(=O)OCc1c(Cl)cc(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	-8.41		Crippen Method
logp	7.544		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3120.00		NIST Webbook
rinpol	3120.00		NIST Webbook
tb	1009.25	K	Joback Method
tc	1235.70	K	Joback Method
tf	635.76	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.88	J/molxK	1009.25	Joback Method
cpg	1120.23	J/molxK	1197.96	Joback Method
cpg	1112.81	J/molxK	1160.22	Joback Method
cpg	1104.10	J/molxK	1122.48	Joback Method
cpg	1094.07	J/molxK	1084.73	Joback Method
cpg	1082.67	J/molxK	1046.99	Joback Method
cpg	1126.38	J/molxK	1235.70	Joback Method
dvisc	0.0000261	Paxs	1009.25	Joback Method

dvisc	0.0000328	Paxs	947.00	Joback Method
dvisc	0.0000426	Paxs	884.75	Joback Method
dvisc	0.0000575	Paxs	822.50	Joback Method
dvisc	0.0000815	Paxs	760.26	Joback Method
dvisc	0.0001231	Paxs	698.01	Joback Method
dvisc	0.0002015	Paxs	635.76	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=U380575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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