

Sebacic acid, isoheptyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C22H31Cl3O4/c1-16(2)10-9-13-28-20(26)11-7-5-3-4-6-8-12-21(27)29-19-15-1
InchiKey:	JSVLIBRRBOZXHR-UHFFFAOYSA-N
Formula:	C22H31Cl3O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	465.84

Physical Properties

Property code	Value	Unit	Source
gf	-288.19	kJ/mol	Joback Method
hf	-837.39	kJ/mol	Joback Method
hfus	60.25	kJ/mol	Joback Method
hvap	99.91	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mvol	348.680	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3157.00		NIST Webbook
tb	1008.81	K	Joback Method
tc	1235.42	K	Joback Method
tf	620.76	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.25	J/molxK	1008.81	Joback Method
cpg	1120.13	J/molxK	1197.65	Joback Method
cpg	1112.84	J/molxK	1159.88	Joback Method
cpg	1104.24	J/molxK	1122.12	Joback Method
cpg	1094.29	J/molxK	1084.35	Joback Method
cpg	1082.97	J/molxK	1046.58	Joback Method
cpg	1126.15	J/molxK	1235.42	Joback Method
dvisc	0.0000237	Paxs	1008.81	Joback Method
dvisc	0.0000302	Paxs	944.13	Joback Method

dvisc	0.0000398	Paxs	879.46	Joback Method
dvisc	0.0000548	Paxs	814.78	Joback Method
dvisc	0.0000798	Paxs	750.11	Joback Method
dvisc	0.0001248	Paxs	685.43	Joback Method
dvisc	0.0002140	Paxs	620.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355200&Units=SI
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

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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