

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

Inchi:	InChI=1S/C23H33Cl3O4/c1-2-3-4-9-12-15-29-21(27)13-10-7-5-6-8-11-14-22(28)30-20-1
InchiKey:	NTPYPJYTLBLRAC-UHFFFAOYSA-N
Formula:	C23H33Cl3O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	479.87

Physical Properties

Property code	Value	Unit	Source
gf	-277.33	kJ/mol	Joback Method
hf	-852.75	kJ/mol	Joback Method
hfus	66.37	kJ/mol	Joback Method
hvap	102.52	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.187		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	3297.00		NIST Webbook
tb	1032.13	K	Joback Method
tc	1263.80	K	Joback Method
tf	647.03	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.08	J/molxK	1032.13	Joback Method
cpg	1143.05	J/molxK	1070.74	Joback Method
cpg	1154.54	J/molxK	1109.35	Joback Method
cpg	1164.59	J/molxK	1147.97	Joback Method
cpg	1173.23	J/molxK	1186.58	Joback Method
cpg	1180.50	J/molxK	1225.19	Joback Method
cpg	1186.45	J/molxK	1263.80	Joback Method
dvisc	0.0001787	Paxs	647.03	Joback Method
dvisc	0.0001081	Paxs	711.21	Joback Method

dvisc	0.0000710	Paxs	775.40	Joback Method
dvisc	0.0000498	Paxs	839.58	Joback Method
dvisc	0.0000367	Paxs	903.76	Joback Method
dvisc	0.0000282	Paxs	967.95	Joback Method
dvisc	0.0000223	Paxs	1032.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355202&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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