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)30-20-17
InchiKey: NTPYPJYTLBLRAC-UHFFFAOYSA-N
Formula: C23H33Cl3O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=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/mol×K	1032.13	Joback Method
cpg	1143.05	J/mol×K	1070.74	Joback Method
cpg	1154.54	J/mol×K	1109.35	Joback Method
cpg	1164.59	J/mol×K	1147.97	Joback Method
cpg	1173.23	J/mol×K	1186.58	Joback Method
cpg	1180.50	J/mol×K	1225.19	Joback Method
cpg	1186.45	J/mol×K	1263.80	Joback Method
dvisc	0.0001787	Pa×s	647.03	Joback Method
dvisc	0.0001081	Pa×s	711.21	Joback Method

dvisc	0.0000710	Pa×s	775.40	Joback Method
dvisc	0.0000498	Pa×s	839.58	Joback Method
dvisc	0.0000367	Pa×s	903.76	Joback Method
dvisc	0.0000282	Pa×s	967.95	Joback Method
dvisc	0.0000223	Pa×s	1032.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:
https://www.chemeo.com/cid/52-265-0/Sebacic-acid-heptyl-2-3-5-trichlorophenyl-ester.pdf
Generated by Cheméo on 2024-10-12 09:03:23.005507553 +0000 UTC m=+3304665.642476816.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.