

Sebacic acid, nonyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C25H37Cl3O4/c1-2-3-4-5-8-11-14-19-31-22(29)15-12-9-6-7-10-13-16-23(30)3
InchiKey:	BDESVEIOWYBVDT-UHFFFAOYSA-N
Formula:	C25H37Cl3O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	507.92

Physical Properties

Property code	Value	Unit	Source
gf	-260.49	kJ/mol	Joback Method
hf	-894.03	kJ/mol	Joback Method
hfus	71.55	kJ/mol	Joback Method
hvap	106.97	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.967		Crippen Method
mvol	390.950	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	3545.00		NIST Webbook
rinpol	3545.00		NIST Webbook
tb	1077.89	K	Joback Method
tc	1323.48	K	Joback Method
tf	669.57	K	Joback Method
vc	1.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.67	J/molxK	1077.89	Joback Method
cpg	1265.04	J/molxK	1118.82	Joback Method
cpg	1276.70	J/molxK	1159.75	Joback Method
cpg	1286.70	J/molxK	1200.69	Joback Method
cpg	1295.11	J/molxK	1241.62	Joback Method
cpg	1301.98	J/molxK	1282.55	Joback Method
cpg	1307.36	J/molxK	1323.48	Joback Method
dvisc	0.0001395	Paxs	669.57	Joback Method

dvisc	0.0000827	Paxs	737.62	Joback Method
dvisc	0.0000536	Paxs	805.68	Joback Method
dvisc	0.0000371	Paxs	873.73	Joback Method
dvisc	0.0000271	Paxs	941.78	Joback Method
dvisc	0.0000207	Paxs	1009.84	Joback Method
dvisc	0.0000163	Paxs	1077.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355268&Units=SI

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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