

Sebacic acid, 2,3-dichlorobenzyl nonyl ester

Inchi: InChI=1S/C26H40Cl2O4/c1-2-3-4-5-8-11-14-20-31-24(29)18-12-9-6-7-10-13-19-25(30)3
InchiKey: HRIAYKGLCJPBAD-UHFFFAOYSA-N
Formula: C26H40Cl2O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 487.50

Physical Properties

Property code	Value	Unit	Source
gf	-230.51	kJ/mol	Joback Method
hf	-887.46	kJ/mol	Joback Method
hfus	70.33	kJ/mol	Joback Method
hvap	104.15	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.451		Crippen Method
mvol	392.800	ml/mol	McGowan Method
pc	867.60	kPa	Joback Method
rinpol	3423.00		NIST Webbook
rinpol	3423.00		NIST Webbook
tb	1058.36	K	Joback Method
tc	1299.87	K	Joback Method
tf	638.40	K	Joback Method
vc	1.530	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.67	J/mol×K	1058.36	Joback Method
cpg	1307.73	J/mol×K	1098.61	Joback Method
cpg	1321.08	J/mol×K	1138.86	Joback Method
cpg	1332.79	J/mol×K	1179.11	Joback Method
cpg	1342.91	J/mol×K	1219.37	Joback Method
cpg	1351.51	J/mol×K	1259.62	Joback Method
cpg	1358.66	J/mol×K	1299.87	Joback Method
dvisc	0.0001697	Paxs	638.40	Joback Method

dvisc	0.0000947	Paxs	708.39	Joback Method
dvisc	0.0000587	Paxs	778.39	Joback Method
dvisc	0.0000394	Paxs	848.38	Joback Method
dvisc	0.0000281	Paxs	918.37	Joback Method
dvisc	0.0000210	Paxs	988.37	Joback Method
dvisc	0.0000163	Paxs	1058.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380608&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

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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