Sebacic acid, 2,5-dichlorobenzyl nonyl ester

Inchi: InChI=1S/C26H40Cl2O4/c1-2-3-4-5-8-11-14-19-31-25(29)15-12-9-6-7-10-13-16-26(30)32
InchiKey: UEQSQXDRSZIGAV-UHFFFAOYSA-N
Formula: C26H40Cl2O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
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
mcvol	392.800	ml/mol	McGowan Method
pc	867.60	kPa	Joback Method
rinpol	3399.00		NIST Webbook
rinpol	3399.00		NIST Webbook
tb	1058.36	K	Joback Method
tc	1299.87	K	Joback Method
tf	638.40	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.67	J/mol×K	1058.36	Joback Method
cpg	1351.51	J/mol×K	1259.62	Joback Method
cpg	1342.91	J/mol×K	1219.37	Joback Method
cpg	1332.79	J/mol×K	1179.11	Joback Method
cpg	1321.08	J/mol×K	1138.86	Joback Method
cpg	1307.73	J/mol×K	1098.61	Joback Method
cpg	1358.66	J/mol×K	1299.87	Joback Method
dvisc	0.0000163	Pa×s	1058.36	Joback Method

dvisc	0.0000210	Pa×s	988.37	Joback Method
dvisc	0.0000281	Pa×s	918.37	Joback Method
dvisc	0.0000394	Pa×s	848.38	Joback Method
dvisc	0.0000587	Pa×s	778.39	Joback Method
dvisc	0.0000947	Pa×s	708.39	Joback Method
dvisc	0.0001697	Pa×s	638.40	Joback Method

Sources

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=U380619&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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