

Sebacic acid, decyl 2,4-dichlorophenethyl ester

Inchi:	InChI=1S/C28H44Cl2O4/c1-2-3-4-5-6-9-12-15-21-33-27(31)16-13-10-7-8-11-14-17-28(32)
InchiKey:	SQZSIKDVPSXPDE-UHFFFAOYSA-N
Formula:	C28H44Cl2O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	515.55

Physical Properties

Property code	Value	Unit	Source
gf	-213.67	kJ/mol	Joback Method
hf	-928.74	kJ/mol	Joback Method
hfus	75.51	kJ/mol	Joback Method
hvap	108.60	kJ/mol	Joback Method
log10ws	-9.74		Crippen Method
logp	8.884		Crippen Method
mvol	420.980	ml/mol	McGowan Method
pc	777.21	kPa	Joback Method
rinpol	3372.00		NIST Webbook
rinpol	3372.00		NIST Webbook
tb	1104.12	K	Joback Method
tc	1364.93	K	Joback Method
tf	660.94	K	Joback Method
vc	1.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.02	J/molxK	1104.12	Joback Method
cpg	1432.66	J/molxK	1147.59	Joback Method
cpg	1446.30	J/molxK	1191.06	Joback Method
cpg	1458.03	J/molxK	1234.52	Joback Method
cpg	1467.93	J/molxK	1277.99	Joback Method
cpg	1476.11	J/molxK	1321.46	Joback Method
cpg	1482.65	J/molxK	1364.93	Joback Method
dvisc	0.0001311	Paxs	660.94	Joback Method

dvisc	0.0000718	Paxs	734.80	Joback Method
dvisc	0.0000439	Paxs	808.67	Joback Method
dvisc	0.0000292	Paxs	882.53	Joback Method
dvisc	0.0000206	Paxs	956.39	Joback Method
dvisc	0.0000153	Paxs	1030.26	Joback Method
dvisc	0.0000119	Paxs	1104.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U416824&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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