

Sebacic acid, 2,5-dichlorobenzyl heptyl ester

Inchi:	InChI=1S/C24H36Cl2O4/c1-2-3-4-9-12-17-29-23(27)13-10-7-5-6-8-11-14-24(28)30-19-20
InchiKey:	NPWGIMLPSHOCNK-UHFFFAOYSA-N
Formula:	C24H36Cl2O4
SMILES:	CCCCCCCC(=O)CCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	459.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.35	kJ/mol	Joback Method
hf	-846.18	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	99.70	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.671		Crippen Method
mvol	364.620	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	3201.00		NIST Webbook
rinpol	3201.00		NIST Webbook
tb	1012.60	K	Joback Method
tc	1239.97	K	Joback Method
tf	615.86	K	Joback Method
vc	1.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.66	J/molxK	1012.60	Joback Method
cpg	1228.05	J/molxK	1202.08	Joback Method
cpg	1219.16	J/molxK	1164.18	Joback Method
cpg	1208.93	J/molxK	1126.29	Joback Method
cpg	1197.29	J/molxK	1088.39	Joback Method
cpg	1184.22	J/molxK	1050.50	Joback Method
cpg	1235.63	J/molxK	1239.97	Joback Method
dvisc	0.0000223	Paxs	1012.60	Joback Method

dvisc	0.0000286	Paxs	946.48	Joback Method
dvisc	0.0000380	Paxs	880.35	Joback Method
dvisc	0.0000528	Paxs	814.23	Joback Method
dvisc	0.0000779	Paxs	748.11	Joback Method
dvisc	0.0001239	Paxs	681.98	Joback Method
dvisc	0.0002177	Paxs	615.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380617&Units=SI
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

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
mccvol:	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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