

Sebacic acid, butyl 2,4-dichlorophenethyl ester

Inchi:	InChI=1S/C22H32Cl2O4/c1-2-3-15-27-21(25)10-8-6-4-5-7-9-11-22(26)28-16-14-18-12-13
InchiKey:	QMSAEDXNXKFLTA-UHFFFAOYSA-N
Formula:	C22H32Cl2O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	431.39

Physical Properties

Property code	Value	Unit	Source
gf	-264.19	kJ/mol	Joback Method
hf	-804.90	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.543		Crippen Method
mvol	336.440	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2892.00		NIST Webbook
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tb	966.84	K	Joback Method
tc	1184.56	K	Joback Method
tf	593.32	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.35	J/molxK	966.84	Joback Method
cpg	1106.10	J/molxK	1148.27	Joback Method
cpg	1097.05	J/molxK	1111.99	Joback Method
cpg	1086.79	J/molxK	1075.70	Joback Method
cpg	1075.27	J/molxK	1039.41	Joback Method
cpg	1062.47	J/molxK	1003.13	Joback Method
cpg	1113.96	J/molxK	1184.56	Joback Method
dvisc	0.0000304	Paxs	966.84	Joback Method

dvisc	0.0000386	Paxs	904.59	Joback Method
dvisc	0.0000510	Paxs	842.33	Joback Method
dvisc	0.0000703	Paxs	780.08	Joback Method
dvisc	0.0001025	Paxs	717.83	Joback Method
dvisc	0.0001606	Paxs	655.57	Joback Method
dvisc	0.0002763	Paxs	593.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416818&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
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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