

Sebacic acid, butyl 4-chloro-2-methylbenzyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-3-4-15-26-21(24)11-9-7-5-6-8-10-12-22(25)27-17-19-13-14-20
InchiKey:	CDYRTRFRUNIRZGU-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1C
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-252.26	kJ/mol	Joback Method
hf	-789.16	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	90.86	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.156		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	929.41	K	Joback Method
tc	1140.08	K	Joback Method
tf	563.40	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.57	J/molxK	929.41	Joback Method
cpg	1038.87	J/molxK	964.52	Joback Method
cpg	1052.89	J/molxK	999.63	Joback Method
cpg	1065.66	J/molxK	1034.75	Joback Method
cpg	1077.20	J/molxK	1069.86	Joback Method
cpg	1087.55	J/molxK	1104.97	Joback Method
cpg	1096.72	J/molxK	1140.08	Joback Method
dvisc	0.0003410	Paxs	563.40	Joback Method

dvisc	0.0001951	Paxs	624.40	Joback Method
dvisc	0.0001233	Paxs	685.40	Joback Method
dvisc	0.0000840	Paxs	746.41	Joback Method
dvisc	0.0000606	Paxs	807.41	Joback Method
dvisc	0.0000458	Paxs	868.41	Joback Method
dvisc	0.0000359	Paxs	929.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380587&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

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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