

Sebacic acid, isohexyl pentafluorobenzyl ester

Inchi:	InChI=1S/C23H31F5O4/c1-15(2)10-9-13-31-17(29)11-7-5-3-4-6-8-12-18(30)32-14-16-19
InchiKey:	FIAIQWPZVQIPRF-UHFFFAOYSA-N
Formula:	C23H31F5O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	466.48

Physical Properties

Property code	Value	Unit	Source
gf	-1237.29	kJ/mol	Joback Method
hf	-1814.30	kJ/mol	Joback Method
hfus	64.87	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.526		Crippen Method
mvol	334.900	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	925.71	K	Joback Method
tc	1135.53	K	Joback Method
tf	570.26	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.30	J/molxK	925.71	Joback Method
cpg	1107.06	J/molxK	960.68	Joback Method
cpg	1121.43	J/molxK	995.65	Joback Method
cpg	1134.43	J/molxK	1030.62	Joback Method
cpg	1146.08	J/molxK	1065.59	Joback Method
cpg	1156.40	J/molxK	1100.56	Joback Method
cpg	1165.39	J/molxK	1135.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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