

Sebacic acid, hexyl pentafluorobenzyl ester

Inchi:	InChI=1S/C23H31F5O4/c1-2-3-4-11-14-31-17(29)12-9-7-5-6-8-10-13-18(30)32-15-16-19
InchiKey:	HVLBLGKCEGIEKV-UHFFFAOYSA-N
Formula:	C23H31F5O4
SMILES:	CCCCCOC(=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	-1234.85	kJ/mol	Joback Method
hf	-1809.02	kJ/mol	Joback Method
hfus	68.40	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	6.670		Crippen Method
mvol	334.900	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	926.15	K	Joback Method
tc	1136.96	K	Joback Method
tf	585.26	K	Joback Method
vc	1.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.84	J/molxK	926.15	Joback Method
cpg	1106.71	J/molxK	961.28	Joback Method
cpg	1121.19	J/molxK	996.42	Joback Method
cpg	1134.29	J/molxK	1031.55	Joback Method
cpg	1146.04	J/molxK	1066.69	Joback Method
cpg	1156.46	J/molxK	1101.82	Joback Method
cpg	1165.55	J/molxK	1136.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354901&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
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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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