

Sebacic acid, isobutyl pentafluorophenyl ester

Inchi:	InChI=1S/C20H25F5O4/c1-12(2)11-28-13(26)9-7-5-3-4-6-8-10-14(27)29-20-18(24)16(22)
InchiKey:	MLQZUYCSYNORDS-UHFFFAOYSA-N
Formula:	C20H25F5O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	424.40

Physical Properties

Property code	Value	Unit	Source
gf	-1262.55	kJ/mol	Joback Method
hf	-1752.38	kJ/mol	Joback Method
hfus	57.10	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.607		Crippen Method
mvol	292.630	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2244.00		NIST Webbook
tb	857.07	K	Joback Method
tc	1049.66	K	Joback Method
tf	536.45	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.14	J/molxK	857.07	Joback Method
cpg	926.58	J/molxK	889.17	Joback Method
cpg	939.96	J/molxK	921.27	Joback Method
cpg	952.29	J/molxK	953.37	Joback Method
cpg	963.58	J/molxK	985.46	Joback Method
cpg	973.83	J/molxK	1017.56	Joback Method
cpg	983.04	J/molxK	1049.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355024&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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