

Succinic acid, phenethyl pentafluorobenzyl ester

Inchi:	InChI=1S/C19H15F5O4/c20-15-12(16(21)18(23)19(24)17(15)22)10-28-14(26)7-6-13(25)
InchiKey:	AWKWYZBURKPZBL-UHFFFAOYSA-N
Formula:	C19H15F5O4
SMILES:	O=C(CCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCCc1ccccc1
Mol. weight [g/mol]:	402.31

Physical Properties

Property code	Value	Unit	Source
gf	-1156.12	kJ/mol	Joback Method
hf	-1489.93	kJ/mol	Joback Method
hfus	52.08	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	3.991		Crippen Method
mvol	254.780	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rmpol	2372.00		NIST Webbook
tb	861.31	K	Joback Method
tc	1063.19	K	Joback Method
tf	566.60	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.49	J/molxK	861.31	Joback Method
cpg	768.06	J/molxK	894.96	Joback Method
cpg	778.61	J/molxK	928.60	Joback Method
cpg	788.16	J/molxK	962.25	Joback Method
cpg	796.72	J/molxK	995.90	Joback Method
cpg	804.29	J/molxK	1029.55	Joback Method
cpg	810.89	J/molxK	1063.19	Joback Method

Sources

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=U358005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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