

Succinic acid, ethyl 2-(pentafluorophenoxy)ethyl ester

Inchi:	InChI=1S/C14H13F5O5/c1-2-22-7(20)3-4-8(21)23-5-6-24-14-12(18)10(16)9(15)11(17)13
InchiKey:	WPPKXCLYCFRFRY-UHFFFAOYSA-N
Formula:	C14H13F5O5
SMILES:	CCOC(=O)CCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	356.24

Physical Properties

Property code	Value	Unit	Source
gf	-1415.63	kJ/mol	Joback Method
hf	-1755.48	kJ/mol	Joback Method
hfus	46.27	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.647		Crippen Method
mcvol	213.960	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	742.65	K	Joback Method
tc	921.94	K	Joback Method
tf	506.06	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.51	J/molxK	742.65	Joback Method
cpg	612.91	J/molxK	772.53	Joback Method
cpg	623.65	J/molxK	802.41	Joback Method
cpg	633.71	J/molxK	832.30	Joback Method
cpg	643.07	J/molxK	862.18	Joback Method
cpg	651.71	J/molxK	892.06	Joback Method
cpg	659.63	J/molxK	921.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381546&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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