

Succinic acid, 2,2,3,3-tetrafluoropropyl pentafluorobenzyl ester

Inchi: InChI=1S/C14H9F9O4/c15-8-5(9(16)11(18)12(19)10(8)17)3-26-6(24)1-2-7(25)27-4-14(22)
InchiKey: FIAASMFUHZQLSN-UHFFFAOYSA-N
Formula: C14H9F9O4
SMILES: O=C(CCC(=O)OCC(F)(F)C(F)F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 412.20

Physical Properties

Property code	Value	Unit	Source
gf	-2089.47	kJ/mol	Joback Method
hf	-2421.73	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	61.62	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.649		Crippen Method
mvol	215.170	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	713.64	K	Joback Method
tc	882.15	K	Joback Method
tf	473.61	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.23	J/molxK	713.64	Joback Method
cpg	620.62	J/molxK	741.73	Joback Method
cpg	630.40	J/molxK	769.81	Joback Method
cpg	639.58	J/molxK	797.90	Joback Method
cpg	648.16	J/molxK	825.98	Joback Method
cpg	656.17	J/molxK	854.07	Joback Method
cpg	663.59	J/molxK	882.15	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=U389877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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