Succinic acid, hexyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C12H19F3O4/c1-2-3-4-5-8-18-10(16)6-7-11(17)19-9-12(13,14)15/h2-9H2,1H3
InchiKey: HXUKNYVIZNJLOI-UHFFFAOYSA-N
Formula: C12H19F3O4
SMILES: CCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 284.27

Physical Properties

Property code	Value	Unit	Source
gf	-999.27	kJ/mol	Joback Method
hf	-1377.69	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.996		Crippen Method
mcvol	200.130	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	621.12	K	Joback Method
tc	787.51	K	Joback Method
tf	373.51	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.13	J/mol×K	621.12	Joback Method
cpg	556.57	J/mol×K	648.85	Joback Method
cpg	569.37	J/mol×K	676.58	Joback Method
cpg	581.56	J/mol×K	704.31	Joback Method
cpg	593.14	J/mol×K	732.04	Joback Method
cpg	604.13	J/mol×K	759.78	Joback Method
cpg	614.53	J/mol×K	787.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382464&Units=SI
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

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume