

Succinic acid, 2-methylhex-3-yl 2,2,2-trifluoroethyl ester

Inchi:	InChI=1S/C13H21F3O4/c1-4-5-10(9(2)3)20-12(18)7-6-11(17)19-8-13(14,15)16/h9-10H,4
InchiKey:	IEROHXWWZOTHJZ-UHFFFAOYSA-N
Formula:	C13H21F3O4
SMILES:	CCCC(OC(=O)CCC(=O)OCC(F)(F)F)C(C)C
Mol. weight [g/mol]:	298.30

Physical Properties

Property code	Value	Unit	Source
gf	-995.73	kJ/mol	Joback Method
hf	-1408.89	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.240		Crippen Method
mvol	214.220	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	643.12	K	Joback Method
tc	813.93	K	Joback Method
tf	354.78	K	Joback Method
vc	0.843	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.03	J/mol×K	643.12	Joback Method
cpg	610.47	J/mol×K	671.59	Joback Method
cpg	624.20	J/mol×K	700.06	Joback Method
cpg	637.22	J/mol×K	728.53	Joback Method
cpg	649.55	J/mol×K	756.99	Joback Method
cpg	661.20	J/mol×K	785.46	Joback Method
cpg	672.20	J/mol×K	813.93	Joback Method

Sources

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=U382463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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