

Succinic acid, 2,2,3,3-tetrafluoropropyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C14H22F4O4/c1-8(2)12(9(3)4)22-11(20)6-5-10(19)21-7-14(17,18)13(15)16/h8
InchiKey: LTRAQBXYJIDCW-UHFFFAOYSA-N
Formula: C14H22F4O4
SMILES: CC(C)C(OC(=O)CCC(=O)OCC(F)(F)C(F)F)C(C)C
Mol. weight [g/mol]: 330.32

Physical Properties

Property code	Value	Unit	Source
gf	-1187.00	kJ/mol	Joback Method
hf	-1636.20	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.434		Crippen Method
mvol	230.080	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	664.39	K	Joback Method
tc	834.32	K	Joback Method
tf	336.64	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.28	J/mol×K	664.39	Joback Method
cpg	673.15	J/mol×K	692.71	Joback Method
cpg	687.25	J/mol×K	721.03	Joback Method
cpg	700.60	J/mol×K	749.35	Joback Method
cpg	713.22	J/mol×K	777.67	Joback Method
cpg	725.11	J/mol×K	806.00	Joback Method
cpg	736.30	J/mol×K	834.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U390499&Units=SI

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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