

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

Inchi: InChI=1S/C12H16F4O5/c13-11(14)12(15,16)7-21-10(18)4-3-9(17)20-6-8-2-1-5-19-8/h8,1
InchiKey: FCJWMEWJVUWCGH-UHFFFAOYSA-N
Formula: C12H16F4O5
SMILES: O=C(CCC(=O)OCC(F)(F)C(F)F)OCC1CCCCO1
Mol. weight [g/mol]: 316.25

Physical Properties

Property code	Value	Unit	Source
gf	-1246.09	kJ/mol	Joback Method
hf	-1650.60	kJ/mol	Joback Method
hfus	35.71	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.932		Crippen Method
mcvol	196.910	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1661.00		NIST Webbook
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tb	662.18	K	Joback Method
tc	843.33	K	Joback Method
tf	396.57	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.04	J/mol×K	662.18	Joback Method
cpg	587.09	J/mol×K	692.37	Joback Method
cpg	600.32	J/mol×K	722.56	Joback Method
cpg	612.73	J/mol×K	752.76	Joback Method
cpg	624.36	J/mol×K	782.95	Joback Method
cpg	635.21	J/mol×K	813.14	Joback Method
cpg	645.32	J/mol×K	843.33	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=U390711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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