

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

Inchi:	InChI=1S/C9H12F4O4/c1-2-16-6(14)3-4-7(15)17-5-9(12,13)8(10)11/h8H,2-5H2,1H3
InchiKey:	IJKKMZYGWNXLBG-UHFFFAOYSA-N
Formula:	C9H12F4O4
SMILES:	CCOC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	260.18

Physical Properties

Property code	Value	Unit	Source
gf	-1221.78	kJ/mol	Joback Method
hf	-1517.16	kJ/mol	Joback Method
hfus	26.02	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.773		Crippen Method
mvol	159.630	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	551.31	K	Joback Method
tc	715.73	K	Joback Method
tf	325.29	K	Joback Method
vc	0.642	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.71	J/molxK	551.31	Joback Method
cpg	415.94	J/molxK	578.71	Joback Method
cpg	426.65	J/molxK	606.12	Joback Method
cpg	436.86	J/molxK	633.52	Joback Method
cpg	446.58	J/molxK	660.92	Joback Method
cpg	455.81	J/molxK	688.32	Joback Method
cpg	464.57	J/molxK	715.73	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=U390859&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
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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