

Succinic acid, 2,2,3,3-tetrafluoropropyl cis-pent-2-en-1-yl ester

Inchi:	InChI=1S/C12H16F4O4/c1-2-3-4-7-19-9(17)5-6-10(18)20-8-12(15,16)11(13)14/h3-4,11H
InchiKey:	BSZDJACDTIWSJB-ARJAWSKDSA-N
Formula:	C12H16F4O4
SMILES:	CCC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	300.25

Physical Properties

Property code	Value	Unit	Source
gf	-1116.30	kJ/mol	Joback Method
hf	-1461.86	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	55.62	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.720		Crippen Method
mvol	197.600	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	624.11	K	Joback Method
tc	792.45	K	Joback Method
tf	354.02	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.85	J/mol×K	624.11	Joback Method
cpg	543.53	J/mol×K	652.17	Joback Method
cpg	555.56	J/mol×K	680.22	Joback Method
cpg	566.97	J/mol×K	708.28	Joback Method
cpg	577.77	J/mol×K	736.34	Joback Method
cpg	587.98	J/mol×K	764.40	Joback Method
cpg	597.62	J/mol×K	792.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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