

Succinic acid, 2,2,3,3-tetrafluoropropyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C15H20F4O4/c1-10-4-2-3-5-11(10)8-22-12(20)6-7-13(21)23-9-15(18,19)14(16)
InchiKey: LFVLQVAIKNHAJA-UHFFFAOYSA-N
Formula: C15H20F4O4
SMILES: CC1=C(COC(=O)CCC(=O)OCC(F)(F)C(F)F)CCCC1
Mol. weight [g/mol]: 340.31

Physical Properties

Property code	Value	Unit	Source
gf	-1128.40	kJ/mol	Joback Method
hf	-1531.50	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.644		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	1863.00		NIST Webbook
rinpol	1863.00		NIST Webbook
tb	721.93	K	Joback Method
tc	907.90	K	Joback Method
tf	430.33	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.54	J/molxK	721.93	Joback Method
cpg	692.37	J/molxK	752.92	Joback Method
cpg	706.28	J/molxK	783.92	Joback Method
cpg	719.30	J/molxK	814.91	Joback Method
cpg	731.44	J/molxK	845.91	Joback Method
cpg	742.72	J/molxK	876.90	Joback Method
cpg	753.17	J/molxK	907.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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