

9-Decen-1-ol, heptafluorobutyrate

Inchi:	InChI=1S/C14H19F7O2/c1-2-3-4-5-6-7-8-9-10-23-11(22)12(15,16)13(17,18)14(19,20)21
InchiKey:	XFATYVOKIPHXML-UHFFFAOYSA-N
Formula:	C14H19F7O2
SMILES:	C=CCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	352.29

Physical Properties

Property code	Value	Unit	Source
gf	-1434.23	kJ/mol	Joback Method
hf	-1850.68	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.279		Crippen Method
mvol	223.650	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	1298.10		NIST Webbook
rinpol	1298.10		NIST Webbook
tb	577.89	K	Joback Method
tc	728.80	K	Joback Method
tf	329.33	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.64	J/mol×K	577.89	Joback Method
cpg	625.07	J/mol×K	603.04	Joback Method
cpg	638.74	J/mol×K	628.19	Joback Method
cpg	651.69	J/mol×K	653.34	Joback Method
cpg	663.93	J/mol×K	678.50	Joback Method
cpg	675.52	J/mol×K	703.65	Joback Method
cpg	686.49	J/mol×K	728.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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