cis-3-Nonen-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C13H17F7O2/c1-2-3-4-5-6-7-8-9-22-10(21)11(14,15)12(16,17)13(18,19)20/h6-
InchiKey: VTEUDUQTJFXMME-SREVYHEPSA-N
Formula: C13H17F7O2
SMILES: CCCCCC=CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 338.26

Physical Properties

Property code	Value	Unit	Source
gf	-1450.27	kJ/mol	Joback Method
hf	-1838.25	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	44.04	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.889		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	1207.40		NIST Webbook
rinpol	1207.40		NIST Webbook
tb	562.49	K	Joback Method
tc	715.98	K	Joback Method
tf	314.74	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.37	J/mol×K	562.49	Joback Method
cpg	575.40	J/mol×K	588.07	Joback Method
cpg	588.65	J/mol×K	613.65	Joback Method
cpg	601.16	J/mol×K	639.24	Joback Method
cpg	612.97	J/mol×K	664.82	Joback Method
cpg	624.12	J/mol×K	690.40	Joback Method
cpg	634.64	J/mol×K	715.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U352764&Units=SI

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

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