2-Norbornanemethanol, heptafluorobutyrate

Inchi: InChI=1S/C12H13F7O2/c13-10(14,11(15,16)12(17,18)19)9(20)21-5-8-4-6-1-2-7(8)3-6/h6
InchiKey: ZWHGCVUKPJCHFO-UHFFFAOYSA-N
Formula: C12H13F7O2
SMILES: O=C(OCC1CC2CCC1C2)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 322.22

Physical Properties

Property code	Value	Unit	Source
gf	-1437.22	kJ/mol	Joback Method
hf	-1815.73	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	41.54	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.799		Crippen Method
mcvol	178.050	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
tb	548.53	K	Joback Method
tc	719.99	K	Joback Method
tf	336.67	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.55	J/mol×K	548.53	Joback Method
cpg	520.73	J/mol×K	577.11	Joback Method
cpg	535.81	J/mol×K	605.68	Joback Method
cpg	549.88	J/mol×K	634.26	Joback Method
cpg	562.98	J/mol×K	662.83	Joback Method
cpg	575.19	J/mol×K	691.41	Joback Method
cpg	586.57	J/mol×K	719.99	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=U376174&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
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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