1,6-Heptadien-4-ol , heptafluorobutyrate

Inchi: InChI=1S/C11H11F7O2/c1-3-5-7(6-4-2)20-8(19)9(12,13)10(14,15)11(16,17)18/h3-4,7H,1
InchiKey: PHJAIHWJRQETNC-UHFFFAOYSA-N
Formula: C11H11F7O2
SMILES: C=CCC(CC=C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 308.19

Physical Properties

Property code	Value	Unit	Source
gf	-1374.09	kJ/mol	Joback Method
hf	-1668.61	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.883		Crippen Method
mcvol	177.080	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	915.60		NIST Webbook
tb	505.49	K	Joback Method
tc	660.65	K	Joback Method
tf	278.76	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.99	J/mol×K	505.49	Joback Method
cpg	456.82	J/mol×K	531.35	Joback Method
cpg	468.88	J/mol×K	557.21	Joback Method
cpg	480.22	J/mol×K	583.07	Joback Method
cpg	490.86	J/mol×K	608.93	Joback Method
cpg	500.83	J/mol×K	634.79	Joback Method
cpg	510.18	J/mol×K	660.65	Joback Method

Sources

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=U352757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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