trans-3-Hexen-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C10H11F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h3-4H,2,5-6H
InchiKey: IIKAVGQGNAGAMG-ONEGZZNKSA-N
Formula: C10H11F7O2
SMILES: CCC=CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 296.18

Physical Properties

Property code	Value	Unit	Source
gf	-1475.53	kJ/mol	Joback Method
hf	-1776.33	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	37.36	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.719		Crippen Method
mcvol	167.290	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	927.10		NIST Webbook
rinpol	927.10		NIST Webbook
tb	493.85	K	Joback Method
tc	647.78	K	Joback Method
tf	280.93	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.08	J/mol×K	493.85	Joback Method
cpg	429.65	J/mol×K	519.50	Joback Method
cpg	441.48	J/mol×K	545.16	Joback Method
cpg	452.60	J/mol×K	570.81	Joback Method
cpg	463.05	J/mol×K	596.47	Joback Method
cpg	472.86	J/mol×K	622.12	Joback Method
cpg	482.07	J/mol×K	647.78	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=U352308&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