2-Ethylcyclohexanol, heptafluorobutyrate

Inchi: InChI=1S/C12H15F7O2/c1-2-7-5-3-4-6-8(7)21-9(20)10(13,14)11(15,16)12(17,18)19/h7-8
InchiKey: QUGSZKGFYRCIMJ-UHFFFAOYSA-N
Formula: C12H15F7O2
SMILES: CCC1CCCCC1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 324.24
CAS: 959079-92-6

Physical Properties

Property code	Value	Unit	Source
gf	-1522.17	kJ/mol	Joback Method
hf	-1900.85	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.331		Crippen Method
mcvol	188.910	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	550.33	K	Joback Method
tc	721.51	K	Joback Method
tf	311.69	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.28	J/mol×K	550.33	Joback Method
cpg	537.25	J/mol×K	578.86	Joback Method
cpg	553.20	J/mol×K	607.39	Joback Method
cpg	568.17	J/mol×K	635.92	Joback Method
cpg	582.20	J/mol×K	664.45	Joback Method
cpg	595.34	J/mol×K	692.98	Joback Method
cpg	607.62	J/mol×K	721.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959079926&Units=SI
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

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