Benzamide, 2-fluoro-N-heptyl-

Inchi: InChI=1S/C14H20FNO/c1-2-3-4-5-8-11-16-14(17)12-9-6-7-10-13(12)15/h6-7,9-10H,2-5,8
InchiKey: QJYXVGDNMHUVFG-UHFFFAOYSA-N
Formula: C14H20FNO
SMILES: CCCCCCCNC(=O)c1ccccc1F
Mol. weight [g/mol]: 237.31

Physical Properties

Property code	Value	Unit	Source
gf	-64.56	kJ/mol	Joback Method
hf	-362.45	kJ/mol	Joback Method
hfus	35.45	kJ/mol	Joback Method
hvap	62.06	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.526		Crippen Method
mcvol	197.680	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	654.69	K	Joback Method
tc	849.61	K	Joback Method
tf	389.66	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.75	J/mol×K	654.69	Joback Method
cpg	545.07	J/mol×K	687.18	Joback Method
cpg	559.52	J/mol×K	719.66	Joback Method
cpg	573.13	J/mol×K	752.15	Joback Method
cpg	585.94	J/mol×K	784.63	Joback Method
cpg	597.98	J/mol×K	817.12	Joback Method
cpg	609.29	J/mol×K	849.61	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=U407137&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