Benzamide, 2-fluoro-N-(hept-2-yl)-

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

Physical Properties

Property code	Value	Unit	Source
gf	-67.00	kJ/mol	Joback Method
hf	-367.73	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.524		Crippen Method
mcvol	197.680	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
tb	654.25	K	Joback Method
tc	852.57	K	Joback Method
tf	374.66	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.21	J/mol×K	654.25	Joback Method
cpg	545.84	J/mol×K	687.30	Joback Method
cpg	560.55	J/mol×K	720.36	Joback Method
cpg	574.39	J/mol×K	753.41	Joback Method
cpg	587.39	J/mol×K	786.46	Joback Method
cpg	599.59	J/mol×K	819.51	Joback Method
cpg	611.02	J/mol×K	852.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407134&Units=SI

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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