

Benzamide, 3-fluoro-N-heptyl-

Inchi:	InChI=1S/C14H20FNO/c1-2-3-4-5-6-10-16-14(17)12-8-7-9-13(15)11-12/h7-9,11H,2-6,10
InchiKey:	GGPJOGKWRMERNB-UHFFFAOYSA-N
Formula:	C14H20FNO
SMILES:	CCCCCCCNC(=O)c1cccc(F)c1
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
mvol	197.680	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	654.69	K	Joback Method
tc	849.61	K	Joback Method
tf	389.66	K	Joback Method
vc	0.770	m ³ /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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407284&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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