Benzamide, 3-fluoro-N-butyl-N-heptyl-

Inchi: InChI=1S/C18H28FNO/c1-3-5-7-8-9-14-20(13-6-4-2)18(21)16-11-10-12-17(19)15-16/h10
InchiKey: NYWKUKFOMXPTBQ-UHFFFAOYSA-N
Formula: C18H28FNO
SMILES: CCCCCCCN(CCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 293.42

Physical Properties

Property code	Value	Unit	Source
gf	-9.49	kJ/mol	Joback Method
hf	-430.95	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	66.57	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.038		Crippen Method
mcvol	254.040	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	708.48	K	Joback Method
tc	894.30	K	Joback Method
tf	414.55	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.70	J/mol×K	708.48	Joback Method
cpg	747.21	J/mol×K	739.45	Joback Method
cpg	763.76	J/mol×K	770.42	Joback Method
cpg	779.39	J/mol×K	801.39	Joback Method
cpg	794.14	J/mol×K	832.36	Joback Method
cpg	808.05	J/mol×K	863.33	Joback Method
cpg	821.17	J/mol×K	894.30	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=U415868&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