Benzamide, 3,4-difluoro-N-heptyl-

Inchi: InChI=1S/C14H19F2NO/c1-2-3-4-5-6-9-17-14(18)11-7-8-12(15)13(16)10-11/h7-8,10H,2-
InchiKey: MRMMODXOOVRURO-UHFFFAOYSA-N
Formula: C14H19F2NO
SMILES: CCCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 255.30

Physical Properties

Property code	Value	Unit	Source
gf	-269.00	kJ/mol	Joback Method
hf	-570.03	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.665		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	658.94	K	Joback Method
tc	847.31	K	Joback Method
tf	402.77	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.22	J/mol×K	658.94	Joback Method
cpg	551.75	J/mol×K	690.34	Joback Method
cpg	565.49	J/mol×K	721.73	Joback Method
cpg	578.47	J/mol×K	753.13	Joback Method
cpg	590.72	J/mol×K	784.52	Joback Method
cpg	602.25	J/mol×K	815.92	Joback Method
cpg	613.11	J/mol×K	847.31	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=U407796&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