Benzamide, 3,4-difluoro-N-hept-2-yl-

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

Physical Properties

Property code	Value	Unit	Source
gf	-271.44	kJ/mol	Joback Method
hf	-575.31	kJ/mol	Joback Method
hfus	34.61	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.663		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	658.50	K	Joback Method
tc	849.96	K	Joback Method
tf	387.77	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.70	J/mol×K	658.50	Joback Method
cpg	552.50	J/mol×K	690.41	Joback Method
cpg	566.48	J/mol×K	722.32	Joback Method
cpg	579.66	J/mol×K	754.23	Joback Method
cpg	592.08	J/mol×K	786.14	Joback Method
cpg	603.76	J/mol×K	818.05	Joback Method
cpg	614.72	J/mol×K	849.96	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=U407793&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