Benzamide, 3-(trifluoromethyl)-N-(hept-2-yl)-

Inchi: InChI=1S/C15H20F3NO/c1-3-4-5-7-11(2)19-14(20)12-8-6-9-13(10-12)15(16,17)18/h6,8-1
InchiKey: LTENOJFTMXIESF-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCCC(C)NC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-445.36	kJ/mol	Joback Method
hf	-789.34	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.404		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	672.44	K	Joback Method
tc	862.76	K	Joback Method
tf	389.53	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.84	J/mol×K	672.44	Joback Method
cpg	617.10	J/mol×K	704.16	Joback Method
cpg	631.41	J/mol×K	735.88	Joback Method
cpg	644.84	J/mol×K	767.60	Joback Method
cpg	657.42	J/mol×K	799.32	Joback Method
cpg	669.22	J/mol×K	831.04	Joback Method
cpg	680.27	J/mol×K	862.76	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=U407170&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