Benzamide, 3-(trifluoromethyl)-N-heptyl-

Inchi: InChI=1S/C15H20F3NO/c1-2-3-4-5-6-10-19-14(20)12-8-7-9-13(11-12)15(16,17)18/h7-9,1
InchiKey: SPCOMULOJZOYFX-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCCCCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-442.92	kJ/mol	Joback Method
hf	-784.06	kJ/mol	Joback Method
hfus	36.78	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.406		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	672.88	K	Joback Method
tc	860.27	K	Joback Method
tf	404.53	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.36	J/mol×K	672.88	Joback Method
cpg	616.35	J/mol×K	704.11	Joback Method
cpg	630.43	J/mol×K	735.34	Joback Method
cpg	643.66	J/mol×K	766.57	Joback Method
cpg	656.09	J/mol×K	797.81	Joback Method
cpg	667.75	J/mol×K	829.04	Joback Method
cpg	678.70	J/mol×K	860.27	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=U407173&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