

Benzamide, 4-(trifluoromethyl)-N-heptyl-

Inchi:	InChI=1S/C15H20F3NO/c1-2-3-4-5-6-11-19-14(20)12-7-9-13(10-8-12)15(16,17)18/h7-10
InchiKey:	HNIXJIFTWPAIKB-UHFFFAOYSA-N
Formula:	C15H20F3NO
SMILES:	CCCCCCCNC(=O)c1ccc(C(F)(F)F)cc1
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
mvol	215.310	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	672.88	K	Joback Method
tc	860.27	K	Joback Method
tf	404.53	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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