Benzamide, 3-fluoro-4-trifluoromethyl-N-heptyl-

Inchi: InChI=1S/C15H19F4NO/c1-2-3-4-5-6-9-20-14(21)11-7-8-12(13(16)10-11)15(17,18)19/h7

InchiKey: BJRGARNKZFCJIL-UHFFFAOYSA-N

Formula: C15H19F4NO

SMILES: CCCCCCCNC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 305.31

Physical Properties

Property code	Value	Unit	Source
gf	-647.36	kJ/mol	Joback Method
hf	-991.64	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.545		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	677.13	K	Joback Method
tc	859.00	K	Joback Method
tf	417.64	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.77	J/mol×K	677.13	Joback Method
cpg	623.05	J/mol×K	707.44	Joback Method
cpg	636.50	J/mol×K	737.75	Joback Method
cpg	649.16	J/mol×K	768.06	Joback Method
cpg	661.07	J/mol×K	798.38	Joback Method
cpg	672.28	J/mol×K	828.69	Joback Method
cpg	682.82	J/mol×K	859.00	Joback Method

Sources

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=U407892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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