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

Inchi: InChI=1S/C15H19F4NO/c1-3-4-5-7-10(2)20-14(21)11-8-6-9-12(13(11)16)15(17,18)19/h6

InchiKey: IIAQURNKXJQPJO-UHFFFAOYSA-N

Formula: C15H19F4NO

SMILES: CCCCCC(C)NC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 305.31

Physical Properties

Property code	Value	Unit	Source
gf	-649.80	kJ/mol	Joback Method
hf	-996.92	kJ/mol	Joback Method
hfus	35.95	kJ/mol	Joback Method
hvap	60.81	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.543		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	676.69	K	Joback Method
tc	861.19	K	Joback Method
tf	402.64	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.26	J/mol×K	676.69	Joback Method
cpg	623.77	J/mol×K	707.44	Joback Method
cpg	637.43	J/mol×K	738.19	Joback Method
cpg	650.26	J/mol×K	768.94	Joback Method
cpg	662.32	J/mol×K	799.69	Joback Method
cpg	673.65	J/mol×K	830.44	Joback Method
cpg	684.28	J/mol×K	861.19	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=U407704&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