

Benzamide, 2,3,4-trifluoro-N-(hept-2-yl)-

Inchi:	InChI=1S/C14H18F3NO/c1-3-4-5-6-9(2)18-14(19)10-7-8-11(15)13(17)12(10)16/h7-9H,3-
InchiKey:	RVRDVFRBRFJVEY-UHFFFAOYSA-N
Formula:	C14H18F3NO
SMILES:	CCCCC(C)NC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]:	273.29

Physical Properties

Property code	Value	Unit	Source
gf	-475.88	kJ/mol	Joback Method
hf	-782.89	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.803		Crippen Method
mvol	201.220	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	662.75	K	Joback Method
tc	848.05	K	Joback Method
tf	400.88	K	Joback Method
vc	0.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.12	J/mol×K	662.75	Joback Method
cpg	559.18	J/mol×K	693.63	Joback Method
cpg	572.49	J/mol×K	724.52	Joback Method
cpg	585.07	J/mol×K	755.40	Joback Method
cpg	596.94	J/mol×K	786.28	Joback Method
cpg	608.14	J/mol×K	817.17	Joback Method
cpg	618.67	J/mol×K	848.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407263&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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