

Benzamide, N,N-diheptyl-2-trifluoromethyl-

Inchi:	InChI=1S/C22H34F3NO/c1-3-5-7-9-13-17-26(18-14-10-8-6-4-2)21(27)19-15-11-12-16-20
InchiKey:	ZSTDGVDWRIYMOE-UHFFFAOYSA-N
Formula:	C22H34F3NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	385.51

Physical Properties

Property code	Value	Unit	Source
gf	-362.59	kJ/mol	Joback Method
hf	-914.48	kJ/mol	Joback Method
hfus	52.83	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.088		Crippen Method
mvol	313.940	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook
tb	795.31	K	Joback Method
tc	979.76	K	Joback Method
tf	463.23	K	Joback Method
vc	1.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.21	J/molxK	795.31	Joback Method
cpg	998.17	J/molxK	826.05	Joback Method
cpg	1015.12	J/molxK	856.79	Joback Method
cpg	1031.11	J/molxK	887.54	Joback Method
cpg	1046.20	J/molxK	918.28	Joback Method
cpg	1060.48	J/molxK	949.02	Joback Method
cpg	1073.98	J/molxK	979.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308536&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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