

Benzamide, N,N-diheptyl-2,3,4-trifluoro-

Inchi:	InChI=1S/C21H32F3NO/c1-3-5-7-9-11-15-25(16-12-10-8-6-4-2)21(26)17-13-14-18(22)20
InchiKey:	KHQJSACENQBMDQ-UHFFFAOYSA-N
Formula:	C21H32F3NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]:	371.48

Physical Properties

Property code	Value	Unit	Source
gf	-393.11	kJ/mol	Joback Method
hf	-908.03	kJ/mol	Joback Method
hfus	56.88	kJ/mol	Joback Method
hvap	72.94	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.487		Crippen Method
mvol	299.850	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2279.00		NIST Webbook
tb	785.62	K	Joback Method
tc	966.93	K	Joback Method
tf	474.58	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.93	J/mol×K	785.62	Joback Method
cpg	936.33	J/mol×K	815.84	Joback Method
cpg	952.78	J/mol×K	846.06	Joback Method
cpg	968.33	J/mol×K	876.27	Joback Method
cpg	983.01	J/mol×K	906.49	Joback Method
cpg	996.86	J/mol×K	936.71	Joback Method
cpg	1009.92	J/mol×K	966.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308423&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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