

Benzamide, N,N-diheptyl-3-fluoro-

Inchi:	InChI=1S/C21H34FNO/c1-3-5-7-9-11-16-23(17-12-10-8-6-4-2)21(24)19-14-13-15-20(22)
InchiKey:	XLDIBWYPPYQHJF-UHFFFAOYSA-N
Formula:	C21H34FNO
SMILES:	CCCCCCCN(CCCCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]:	335.50

Physical Properties

Property code	Value	Unit	Source
gf	15.77	kJ/mol	Joback Method
hf	-492.87	kJ/mol	Joback Method
hfus	51.50	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.209		Crippen Method
mvol	296.310	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	777.12	K	Joback Method
tc	963.23	K	Joback Method
tf	448.36	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.17	J/molxK	777.12	Joback Method
cpg	922.53	J/molxK	808.14	Joback Method
cpg	939.87	J/molxK	839.16	Joback Method
cpg	956.24	J/molxK	870.17	Joback Method
cpg	971.68	J/molxK	901.19	Joback Method
cpg	986.25	J/molxK	932.21	Joback Method
cpg	1000.00	J/molxK	963.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/43-118-3/Benzamide-N-N-diheptyl-3-fluoro.pdf>

Generated by Cheméo on 2024-04-17 02:41:46.53558364 +0000 UTC m=+15610955.456161003.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.