

Benzamide, 2,6-difluoro-3-methyl-N-hept-2-yl-

Inchi:	InChI=1S/C15H21F2NO/c1-4-5-6-7-11(3)18-15(19)13-12(16)9-8-10(2)14(13)17/h8-9,11H
InchiKey:	QGWRWAPNUKGGPP-UHFFFAOYSA-N
Formula:	C15H21F2NO
SMILES:	CCCCC(C)NC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]:	269.33

Physical Properties

Property code	Value	Unit	Source
gf	-272.65	kJ/mol	Joback Method
hf	-607.42	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	3.972		Crippen Method
mvol	213.540	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	686.36	K	Joback Method
tc	877.00	K	Joback Method
tf	411.56	K	Joback Method
vc	0.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.19	J/mol×K	686.36	Joback Method
cpg	605.29	J/mol×K	718.13	Joback Method
cpg	619.58	J/mol×K	749.91	Joback Method
cpg	633.06	J/mol×K	781.68	Joback Method
cpg	645.77	J/mol×K	813.46	Joback Method
cpg	657.73	J/mol×K	845.23	Joback Method
cpg	668.97	J/mol×K	877.00	Joback Method

Sources

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=U407740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/114-492-9/Benzamide-2-6-difluoro-3-methyl-N-hept-2-yl.pdf>

Generated by Cheméo on 2024-04-28 17:28:53.680302824 +0000 UTC m=+16614582.600880144.

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