

Benzamide, 2,6-difluoro-3-methyl-N-(2,6-difluoro-3-methylbenzyl)

Inchi:	InChI=1S/C19H17F4NO2/c1-4-9-24(18(25)14-12(20)7-5-10(2)16(14)22)19(26)15-13(21)2
InchiKey:	LABXQPIEUIGFKN-UHFFFAOYSA-N
Formula:	C19H17F4NO2
SMILES:	CCCN(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]:	367.34

Physical Properties

Property code	Value	Unit	Source
gf	-650.16	kJ/mol	Joback Method
hf	-973.32	kJ/mol	Joback Method
hfus	49.25	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	4.552		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2209.00		NIST Webbook
rinpol	2209.00		NIST Webbook
tb	834.62	K	Joback Method
tc	1039.50	K	Joback Method
tf	566.54	K	Joback Method
vc	0.986	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.32	J/molxK	834.62	Joback Method
cpg	748.04	J/molxK	868.77	Joback Method
cpg	759.83	J/molxK	902.91	Joback Method
cpg	770.73	J/molxK	937.06	Joback Method
cpg	780.78	J/molxK	971.21	Joback Method
cpg	790.01	J/molxK	1005.35	Joback Method
cpg	798.46	J/molxK	1039.50	Joback Method

Sources

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=U407754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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/118-420-4/Benzamide-2-6-difluoro-3-methyl-N-2-6-difluoro-3-methylbenzoyl-N-propyl.p>

Generated by Cheméo on 2024-05-08 04:18:18.034389052 +0000 UTC m=+17431146.954966370.

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