

Benzamide, 3-fluoro-5-trifluoromethyl-N-(3-fluoro-5-trifluoromethyl)

Inchi: InChI=1S/C24H23F8NO2/c1-2-3-4-5-6-7-10-33(21(34)15-11-16(23(27,28)29)13-18(26)12)/h1-10,12-14,16-18,20,22,24,26,28,30,32,34/t1-10,12-14,16-18,20,22,24,26,28,30,32,34/b1-10,12-14,16-18,20,22,24,26,28,30,32,34

InchiKey: HXPMPQPNFRQVKO-UHFFFAOYSA-N

Formula: C24H23F8NO2

SMILES: CCCCCCCN(C(=O)c1cc(F)cc(C(F)(F)F)c1)C(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 509.43

Physical Properties

Property code	Value	Unit	Source
gf	-1362.36	kJ/mol	Joback Method
hf	-1855.52	kJ/mol	Joback Method
hfus	60.47	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	7.646		Crippen Method
mcvol	328.780	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	929.68	K	Joback Method
tc	1138.24	K	Joback Method
tf	605.05	K	Joback Method
vc	1.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.43	J/molxK	929.68	Joback Method
cpg	1070.96	J/molxK	964.44	Joback Method
cpg	1083.59	J/molxK	999.20	Joback Method
cpg	1095.43	J/molxK	1033.96	Joback Method
cpg	1106.59	J/molxK	1068.72	Joback Method
cpg	1117.19	J/molxK	1103.48	Joback Method
cpg	1127.33	J/molxK	1138.24	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=U407877&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
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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