

Benzamide, 3-trifluoromethyl-2-fluoro-N-(3-trifluoromethyl-2-fluorophenyl)

Inchi: InChI=1S/C34H43F8NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-43(31(44)25-26-27-28-29-30-32-33)/n1
InchiKey: VICDHFSUZXTMB-UHFFFAOYSA-N
Formula: C34H43F8NO2
SMILES: CCCCCCCCCCCCCCCCCCN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 649.70

Physical Properties

Property code	Value	Unit	Source
gf	-1278.16	kJ/mol	Joback Method
hf	-2061.92	kJ/mol	Joback Method
hfus	86.37	kJ/mol	Joback Method
hvap	104.88	kJ/mol	Joback Method
log10ws	-13.57		Crippen Method
logp	11.547		Crippen Method
mcvol	469.680	ml/mol	McGowan Method
pc	601.32	kPa	Joback Method
rinpola	3336.00		NIST Webbook
rinpola	3336.00		NIST Webbook
tb	1158.48	K	Joback Method
tc	1478.94	K	Joback Method
tf	717.75	K	Joback Method
vc	1.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1679.45	J/molxK	1158.48	Joback Method
cpg	1702.83	J/molxK	1211.89	Joback Method
cpg	1725.29	J/molxK	1265.30	Joback Method
cpg	1747.34	J/molxK	1318.71	Joback Method
cpg	1769.48	J/molxK	1372.12	Joback Method
cpg	1792.23	J/molxK	1425.53	Joback Method
cpg	1816.08	J/molxK	1478.94	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=U407732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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