Benzamide, 3-trifluoromethyl-2-fluoro-N-(3-trifluoromethyl-2-fl

Inchi: InChI=1S/C32H39F8NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-41(29(42)23-18-16-2

InchiKey: QONXEFXLVRUPHE-UHFFFAOYSA-N

Formula: C32H39F8NO2

SMILES: CCCCCCCCCCCCCCCCN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 621.64

Physical Properties

Property code	Value	Unit	Source
gf	-1295.00	kJ/mol	Joback Method
hf	-2020.64	kJ/mol	Joback Method
hfus	81.19	kJ/mol	Joback Method
hvap	100.43	kJ/mol	Joback Method
log10ws	-12.73		Crippen Method
logp	10.766		Crippen Method
mcvol	441.500	ml/mol	McGowan Method
pc	662.21	kPa	Joback Method
rinpol	3128.00		NIST Webbook
tb	1112.72	K	Joback Method
tc	1398.38	K	Joback Method
tf	695.21	K	Joback Method
vc	1.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1550.64	J/mol×K	1112.72	Joback Method
cpg	1570.94	J/mol×K	1160.33	Joback Method
cpg	1590.25	J/mol×K	1207.94	Joback Method
cpg	1608.91	J/mol×K	1255.55	Joback Method
cpg	1627.25	J/mol×K	1303.16	Joback Method
cpg	1645.62	J/mol×K	1350.77	Joback Method
cpg	1664.36	J/mol×K	1398.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U407731&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume