Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-hexadecyl-

Inchi: InChI=1S/C29H47F4NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-24-34(23-18-6-4-2)28

InchiKey: AGKFMYXIYVIYDF-UHFFFAOYSA-N

Formula: C29H47F4NO

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

Mol. weight [g/mol]: 501.68

Physical Properties

Property code	Value	Unit	Source
gf	-508.09	kJ/mol	Joback Method
hf	-1266.54	kJ/mol	Joback Method
hfus	73.66	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-11.00		Crippen Method
logp	9.958		Crippen Method
mcvol	414.340	ml/mol	McGowan Method
pc	692.16	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	959.72	K	Joback Method
tc	1183.85	K	Joback Method
tf	555.23	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.20	J/mol×K	959.72	Joback Method
cpg	1446.01	J/mol×K	997.08	Joback Method
cpg	1466.46	J/mol×K	1034.43	Joback Method
cpg	1485.67	J/mol×K	1071.79	Joback Method
cpg	1503.80	J/mol×K	1109.14	Joback Method
cpg	1520.96	J/mol×K	1146.50	Joback Method
cpg	1537.29	J/mol×K	1183.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416702&Units=SI
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

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