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

Inchi: InChI=1S/C31H51F4NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-26-36(25-20-6-

InchiKey: RLYMOOPPFKNNBY-UHFFFAOYSA-N

Formula: C31H51F4NO

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

Mol. weight [g/mol]: 529.74

Physical Properties

Property code	Value	Unit	Source
gf	-491.25	kJ/mol	Joback Method
hf	-1307.82	kJ/mol	Joback Method
hfus	78.84	kJ/mol	Joback Method
hvap	92.42	kJ/mol	Joback Method
log10ws	-11.84		Crippen Method
logp	10.738		Crippen Method
mcvol	442.520	ml/mol	McGowan Method
pc	627.19	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
tb	1005.48	K	Joback Method
tc	1251.64	K	Joback Method
tf	577.77	K	Joback Method
vc	1.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.15	J/mol×K	1005.48	Joback Method
cpg	1577.94	J/mol×K	1046.51	Joback Method
cpg	1600.19	J/mol×K	1087.53	Joback Method
cpg	1621.07	J/mol×K	1128.56	Joback Method
cpg	1640.80	J/mol×K	1169.59	Joback Method
cpg	1659.54	J/mol×K	1210.62	Joback Method
cpg	1677.49	J/mol×K	1251.64	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=U416703&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