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

Inchi: InChI=1S/C21H31F4NO/c1-4-7-9-14-26(15-16(6-3)11-8-5-2)20(27)17-12-10-13-18(19(17

InchiKey: AUHBPCKHTJUAFJ-UHFFFAOYSA-N

Formula: C21H31F4NO

SMILES: CCCCCN(CC(CC)CCCC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 389.47

Physical Properties

Property code	Value	Unit	Source
gf	-577.89	kJ/mol	Joback Method
hf	-1106.70	kJ/mol	Joback Method
hfus	49.41	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.693		Crippen Method
mcvol	301.620	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	776.24	K	Joback Method
tc	957.88	K	Joback Method
tf	450.07	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.50	J/mol×K	776.24	Joback Method
cpg	945.79	J/mol×K	806.51	Joback Method
cpg	962.10	J/mol×K	836.79	Joback Method
cpg	977.48	J/mol×K	867.06	Joback Method
cpg	991.99	J/mol×K	897.33	Joback Method
cpg	1005.68	J/mol×K	927.61	Joback Method
cpg	1018.62	J/mol×K	957.88	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=U416694&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume