Benzamide, 3,4-difluoro-N-octadecyl-

Inchi: InChI=1S/C25H41F2NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-28-25(29)22-18
InchiKey: HAVZZCZIEAFAEA-UHFFFAOYSA-N
Formula: C25H41F2NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
gf	-176.38	kJ/mol	Joback Method
hf	-797.07	kJ/mol	Joback Method
hfus	66.63	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-9.60		Crippen Method
logp	7.956		Crippen Method
mcvol	354.440	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	910.62	K	Joback Method
tc	1114.99	K	Joback Method
tf	526.74	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.26	J/mol×K	910.62	Joback Method
cpg	1196.25	J/mol×K	944.68	Joback Method
cpg	1214.03	J/mol×K	978.74	Joback Method
cpg	1230.68	J/mol×K	1012.81	Joback Method
cpg	1246.25	J/mol×K	1046.87	Joback Method
cpg	1260.82	J/mol×K	1080.93	Joback Method
cpg	1274.46	J/mol×K	1114.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407804&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