Benzamide, 3,4-difluoro-N-tetradecyl-

Inchi: InChI=1S/C21H33F2NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-24-21(25)18-14-15-19(22)20
InchiKey: HHLBOTVBXGFQOR-UHFFFAOYSA-N
Formula: C21H33F2NO
SMILES: CCCCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 353.49

Physical Properties

Property code	Value	Unit	Source
gf	-210.06	kJ/mol	Joback Method
hf	-714.51	kJ/mol	Joback Method
hfus	56.27	kJ/mol	Joback Method
hvap	77.49	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.396		Crippen Method
mcvol	298.080	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	819.10	K	Joback Method
tc	1008.10	K	Joback Method
tf	481.66	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.01	J/mol×K	819.10	Joback Method
cpg	949.24	J/mol×K	850.60	Joback Method
cpg	965.48	J/mol×K	882.10	Joback Method
cpg	980.77	J/mol×K	913.60	Joback Method
cpg	995.15	J/mol×K	945.10	Joback Method
cpg	1008.67	J/mol×K	976.60	Joback Method
cpg	1021.37	J/mol×K	1008.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407802&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