Benzamide, 4-(trifluoromethyl)-N-octadecyl-

Inchi: InChI=1S/C26H42F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-30-25(31)23-18
InchiKey: NZAPHYINIOCYBS-UHFFFAOYSA-N
Formula: C26H42F3NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 441.61

Physical Properties

Property code	Value	Unit	Source
gf	-350.30	kJ/mol	Joback Method
hf	-1011.10	kJ/mol	Joback Method
hfus	65.27	kJ/mol	Joback Method
hvap	85.84	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	8.697		Crippen Method
mcvol	370.300	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
rinpol	3038.00		NIST Webbook
rinpol	3038.00		NIST Webbook
tb	924.56	K	Joback Method
tc	1132.58	K	Joback Method
tf	528.50	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1247.30	J/mol×K	924.56	Joback Method
cpg	1266.56	J/mol×K	959.23	Joback Method
cpg	1284.65	J/mol×K	993.90	Joback Method
cpg	1301.66	J/mol×K	1028.57	Joback Method
cpg	1317.70	J/mol×K	1063.24	Joback Method
cpg	1332.87	J/mol×K	1097.91	Joback Method
cpg	1347.25	J/mol×K	1132.58	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=U407311&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

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