Benzamide, 2,5-di(trifluoromethyl)-N-octadecyl-

Inchi: InChI=1S/C27H41F6NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-34-25(35)23-21

InchiKey: ODFYJBAMFCJWBB-UHFFFAOYSA-N

Formula: C27H41F6NO

SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 509.61

Physical Properties

Property code	Value	Unit	Source
gf	-933.10	kJ/mol	Joback Method
hf	-1640.29	kJ/mol	Joback Method
hfus	69.30	kJ/mol	Joback Method
hvap	84.98	kJ/mol	Joback Method
log10ws	-11.14		Crippen Method
logp	9.716		Crippen Method
mcvol	389.700	ml/mol	McGowan Method
pc	744.48	kPa	Joback Method
rinpol	2824.00		NIST Webbook
tb	947.00	K	Joback Method
tc	1165.97	K	Joback Method
tf	556.48	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1330.80	J/mol×K	947.00	Joback Method
cpg	1350.46	J/mol×K	983.50	Joback Method
cpg	1368.93	J/mol×K	1019.99	Joback Method
cpg	1386.36	J/mol×K	1056.49	Joback Method
cpg	1402.87	J/mol×K	1092.98	Joback Method
cpg	1418.62	J/mol×K	1129.48	Joback Method
cpg	1433.73	J/mol×K	1165.97	Joback Method

Sources

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=U407932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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