Benzamide, 2,3,4-trifluoro-N-octadecyl-

Inchi: InChI=1S/C25H40F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-29-25(30)21-18
InchiKey: VJMPTDXPPMKDEH-UHFFFAOYSA-N
Formula: C25H40F3NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 427.59

Physical Properties

Property code	Value	Unit	Source
gf	-380.82	kJ/mol	Joback Method
hf	-1004.65	kJ/mol	Joback Method
hfus	69.32	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-9.93		Crippen Method
logp	8.095		Crippen Method
mcvol	356.210	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	914.87	K	Joback Method
tc	1121.08	K	Joback Method
tf	539.85	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1184.05	J/mol×K	914.87	Joback Method
cpg	1202.93	J/mol×K	949.24	Joback Method
cpg	1220.57	J/mol×K	983.61	Joback Method
cpg	1237.06	J/mol×K	1017.98	Joback Method
cpg	1252.44	J/mol×K	1052.34	Joback Method
cpg	1266.79	J/mol×K	1086.71	Joback Method
cpg	1280.16	J/mol×K	1121.08	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=U407273&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