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

Inchi: InChI=1S/C29H48F3NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-33(23-6-4-2
InchiKey: ULEXFZCBZYIQLZ-UHFFFAOYSA-N
Formula: C29H48F3NO
SMILES: CCCCCCCCCCCCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 483.69

Physical Properties

Property code	Value	Unit	Source
gf	-325.75	kJ/mol	Joback Method
hf	-1073.15	kJ/mol	Joback Method
hfus	77.60	kJ/mol	Joback Method
hvap	90.75	kJ/mol	Joback Method
log10ws	-10.98		Crippen Method
logp	9.608		Crippen Method
mcvol	412.570	ml/mol	McGowan Method
pc	696.18	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	968.66	K	Joback Method
tc	1196.62	K	Joback Method
tf	564.74	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.73	J/mol×K	968.66	Joback Method
cpg	1439.84	J/mol×K	1006.65	Joback Method
cpg	1460.41	J/mol×K	1044.65	Joback Method
cpg	1479.57	J/mol×K	1082.64	Joback Method
cpg	1497.40	J/mol×K	1120.63	Joback Method
cpg	1514.03	J/mol×K	1158.63	Joback Method
cpg	1529.56	J/mol×K	1196.62	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=U415692&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