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

Inchi: InChI=1S/C19H28F3NO/c1-2-3-4-5-6-7-8-9-10-11-14-23-19(24)15-12-13-16(20)18(22)17
InchiKey: STYSMSOZSDYLKZ-UHFFFAOYSA-N
Formula: C19H28F3NO
SMILES: CCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 343.43

Physical Properties

Property code	Value	Unit	Source
gf	-431.34	kJ/mol	Joback Method
hf	-880.81	kJ/mol	Joback Method
hfus	53.78	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	5.755		Crippen Method
mcvol	271.670	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	777.59	K	Joback Method
tc	960.71	K	Joback Method
tf	472.23	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.24	J/mol×K	777.59	Joback Method
cpg	837.26	J/mol×K	808.11	Joback Method
cpg	852.39	J/mol×K	838.63	Joback Method
cpg	866.67	J/mol×K	869.15	Joback Method
cpg	880.14	J/mol×K	899.67	Joback Method
cpg	892.82	J/mol×K	930.19	Joback Method
cpg	904.74	J/mol×K	960.71	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=U407270&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