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

Inchi: InChI=1S/C18H26F3NO/c1-2-3-4-5-6-7-8-9-10-13-22-18(23)14-11-12-15(19)17(21)16(14
InchiKey: MNWCCULZLRWFIZ-UHFFFAOYSA-N
Formula: C18H26F3NO
SMILES: CCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 329.40

Physical Properties

Property code	Value	Unit	Source
gf	-439.76	kJ/mol	Joback Method
hf	-860.17	kJ/mol	Joback Method
hfus	51.19	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.365		Crippen Method
mcvol	257.580	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	754.71	K	Joback Method
tc	936.62	K	Joback Method
tf	460.96	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.72	J/mol×K	754.71	Joback Method
cpg	779.33	J/mol×K	785.03	Joback Method
cpg	794.09	J/mol×K	815.35	Joback Method
cpg	808.03	J/mol×K	845.66	Joback Method
cpg	821.19	J/mol×K	875.98	Joback Method
cpg	833.60	J/mol×K	906.30	Joback Method
cpg	845.27	J/mol×K	936.62	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=U407269&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