Benzamide, 3-(trifluoromethyl)-N-decyl-

Inchi: InChI=1S/C18H26F3NO/c1-2-3-4-5-6-7-8-9-13-22-17(23)15-11-10-12-16(14-15)18(19,20
InchiKey: LPZNWGPLDSRRBP-UHFFFAOYSA-N
Formula: C18H26F3NO
SMILES: CCCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 329.40

Physical Properties

Property code	Value	Unit	Source
gf	-417.66	kJ/mol	Joback Method
hf	-845.98	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	68.04	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.576		Crippen Method
mcvol	257.580	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	741.52	K	Joback Method
tc	926.83	K	Joback Method
tf	438.34	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.54	J/mol×K	741.52	Joback Method
cpg	782.54	J/mol×K	772.40	Joback Method
cpg	797.60	J/mol×K	803.29	Joback Method
cpg	811.77	J/mol×K	834.17	Joback Method
cpg	825.12	J/mol×K	865.06	Joback Method
cpg	837.69	J/mol×K	895.94	Joback Method
cpg	849.53	J/mol×K	926.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U407176&Units=SI

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