Benzamide, 2-(trifluoromethyl)-N-dodecyl-

Inchi: InChI=1S/C20H30F3NO/c1-2-3-4-5-6-7-8-9-10-13-16-24-19(25)17-14-11-12-15-18(17)20
InchiKey: WJVDZOAKEKAFMR-UHFFFAOYSA-N
Formula: C20H30F3NO
SMILES: CCCCCCCCCCCCNC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 357.45

Physical Properties

Property code	Value	Unit	Source
gf	-400.82	kJ/mol	Joback Method
hf	-887.26	kJ/mol	Joback Method
hfus	49.73	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.356		Crippen Method
mcvol	285.760	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	787.28	K	Joback Method
tc	973.86	K	Joback Method
tf	460.88	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.85	J/mol×K	787.28	Joback Method
cpg	898.48	J/mol×K	818.38	Joback Method
cpg	914.15	J/mol×K	849.47	Joback Method
cpg	928.90	J/mol×K	880.57	Joback Method
cpg	942.81	J/mol×K	911.66	Joback Method
cpg	955.92	J/mol×K	942.76	Joback Method
cpg	968.30	J/mol×K	973.86	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=U407196&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