Benzamide, 2,5-di(trifluoromethyl)-N-dodecyl-

Inchi: InChI=1S/C21H29F6NO/c1-2-3-4-5-6-7-8-9-10-11-14-28-19(29)17-15-16(20(22,23)24)12
InchiKey: QRVNQEHEIMZZEJ-UHFFFAOYSA-N
Formula: C21H29F6NO
SMILES: CCCCCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 425.45

Physical Properties

Property code	Value	Unit	Source
gf	-983.62	kJ/mol	Joback Method
hf	-1516.45	kJ/mol	Joback Method
hfus	53.76	kJ/mol	Joback Method
hvap	71.63	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.375		Crippen Method
mcvol	305.160	ml/mol	McGowan Method
pc	1048.01	kPa	Joback Method
rinpol	2238.00		NIST Webbook
tb	809.72	K	Joback Method
tc	993.84	K	Joback Method
tf	488.86	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.99	J/mol×K	809.72	Joback Method
cpg	979.95	J/mol×K	840.41	Joback Method
cpg	994.97	J/mol×K	871.09	Joback Method
cpg	1009.12	J/mol×K	901.78	Joback Method
cpg	1022.48	J/mol×K	932.47	Joback Method
cpg	1035.11	J/mol×K	963.16	Joback Method
cpg	1047.07	J/mol×K	993.84	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=U407929&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