Benzamide, 6-trifluoromethyl-2-fluoro-N-dodecyl-

Inchi: InChI=1S/C20H29F4NO/c1-2-3-4-5-6-7-8-9-10-11-15-25-19(26)18-16(20(22,23)24)13-12

InchiKey: GBLVYKQIMIQCEI-UHFFFAOYSA-N

Formula: C20H29F4NO

SMILES: CCCCCCCCCCCCNC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 375.44

Physical Properties

Property code	Value	Unit	Source
gf	-605.26	kJ/mol	Joback Method
hf	-1094.84	kJ/mol	Joback Method
hfus	52.42	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.495		Crippen Method
mcvol	287.530	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	791.53	K	Joback Method
tc	975.67	K	Joback Method
tf	473.99	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.97	J/mol×K	791.53	Joback Method
cpg	905.14	J/mol×K	822.22	Joback Method
cpg	920.39	J/mol×K	852.91	Joback Method
cpg	934.76	J/mol×K	883.60	Joback Method
cpg	948.30	J/mol×K	914.29	Joback Method
cpg	961.08	J/mol×K	944.98	Joback Method
cpg	973.13	J/mol×K	975.67	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=U407782&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