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

Inchi: InChI=1S/C13H13F6NO/c1-2-3-6-20-11(21)9-7-8(12(14,15)16)4-5-10(9)13(17,18)19/h4-5
InchiKey: WAFAFZDLZFKXKK-UHFFFAOYSA-N
Formula: C13H13F6NO
SMILES: CCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 313.24

Physical Properties

Property code	Value	Unit	Source
gf	-1050.98	kJ/mol	Joback Method
hf	-1351.33	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.254		Crippen Method
mcvol	192.440	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	626.68	K	Joback Method
tc	805.38	K	Joback Method
tf	398.70	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.13	J/mol×K	626.68	Joback Method
cpg	536.91	J/mol×K	656.46	Joback Method
cpg	548.87	J/mol×K	686.25	Joback Method
cpg	560.05	J/mol×K	716.03	Joback Method
cpg	570.50	J/mol×K	745.81	Joback Method
cpg	580.26	J/mol×K	775.60	Joback Method
cpg	589.39	J/mol×K	805.38	Joback Method

Sources

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=U407918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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