

Benzamide, 4-(trifluoromethyl)-N-butyl-N-octyl-

Inchi:	InChI=1S/C20H30F3NO/c1-3-5-7-8-9-10-16-24(15-6-4-2)19(25)17-11-13-18(14-12-17)20
InchiKey:	YAROWDOEYWKEKP-UHFFFAOYSA-N
Formula:	C20H30F3NO
SMILES:	CCCCCCCCN(CCCC)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	357.45

Physical Properties

Property code	Value	Unit	Source
gf	-379.43	kJ/mol	Joback Method
hf	-873.20	kJ/mol	Joback Method
hfus	47.65	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.308		Crippen Method
mvol	285.760	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	749.55	K	Joback Method
tc	931.20	K	Joback Method
tf	440.69	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.95	J/mol×K	749.55	Joback Method
cpg	879.28	J/mol×K	779.83	Joback Method
cpg	895.63	J/mol×K	810.10	Joback Method
cpg	911.05	J/mol×K	840.38	Joback Method
cpg	925.60	J/mol×K	870.65	Joback Method
cpg	939.34	J/mol×K	900.93	Joback Method
cpg	952.32	J/mol×K	931.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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