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

Inchi: InChI=1S/C25H37F6NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-32-23(33)21-19-20(24

InchiKey: KBJIBJRHDNWYDU-UHFFFAOYSA-N

Formula: C25H37F6NO

SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 481.56

Physical Properties

Property code	Value	Unit	Source
gf	-949.94	kJ/mol	Joback Method
hf	-1599.01	kJ/mol	Joback Method
hfus	64.12	kJ/mol	Joback Method
hvap	80.53	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	8.935		Crippen Method
mcvol	361.520	ml/mol	McGowan Method
pc	829.07	kPa	Joback Method
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook
tb	901.24	K	Joback Method
tc	1104.60	K	Joback Method
tf	533.94	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.82	J/mol×K	901.24	Joback Method
cpg	1223.96	J/mol×K	935.13	Joback Method
cpg	1241.02	J/mol×K	969.03	Joback Method
cpg	1257.11	J/mol×K	1002.92	Joback Method
cpg	1272.34	J/mol×K	1036.81	Joback Method
cpg	1286.79	J/mol×K	1070.70	Joback Method
cpg	1300.58	J/mol×K	1104.60	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=U407931&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