

Benzamide, N,N-diundecyl-3-trifluoromethyl-

Inchi:	InChI=1S/C30H50F3NO/c1-3-5-7-9-11-13-15-17-19-24-34(25-20-18-16-14-12-10-8-6-4-2
InchiKey:	OWUZEGLLPBQHB-UHFFFAOYSA-N
Formula:	C30H50F3NO
SMILES:	CCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	497.72

Physical Properties

Property code	Value	Unit	Source
gf	-295.23	kJ/mol	Joback Method
hf	-1079.60	kJ/mol	Joback Method
hfus	73.55	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-11.09		Crippen Method
logp	10.209		Crippen Method
mvol	426.660	ml/mol	McGowan Method
pc	679.23	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	978.35	K	Joback Method
tc	1207.23	K	Joback Method
tf	553.39	K	Joback Method
vc	1.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.24	J/molxK	978.35	Joback Method
cpg	1504.79	J/molxK	1016.50	Joback Method
cpg	1525.96	J/molxK	1054.64	Joback Method
cpg	1545.91	J/molxK	1092.79	Joback Method
cpg	1564.79	J/molxK	1130.94	Joback Method
cpg	1582.75	J/molxK	1169.09	Joback Method
cpg	1599.94	J/molxK	1207.23	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=U308233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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