

Benzamide, N,N-didecyl-3-fluoro-

Inchi: InChI=1S/C27H46FNO/c1-3-5-7-9-11-13-15-17-22-29(23-18-16-14-12-10-8-6-4-2)27(30)
InchiKey: KIAUCYKTJAMNKG-UHFFFAOYSA-N
Formula: C27H46FNO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 419.66

Physical Properties

Property code	Value	Unit	Source
gf	66.29	kJ/mol	Joback Method
hf	-616.71	kJ/mol	Joback Method
hfus	67.04	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-9.48		Crippen Method
logp	8.549		Crippen Method
mcvol	380.850	ml/mol	McGowan Method
pc	826.69	kPa	Joback Method
rinpol	2957.00		NIST Webbook
rinpol	2957.00		NIST Webbook
tb	914.40	K	Joback Method
tc	1119.72	K	Joback Method
tf	515.98	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.42	J/mol×K	914.40	Joback Method
cpg	1296.11	J/mol×K	948.62	Joback Method
cpg	1315.54	J/mol×K	982.84	Joback Method
cpg	1333.80	J/mol×K	1017.06	Joback Method
cpg	1350.95	J/mol×K	1051.28	Joback Method
cpg	1367.09	J/mol×K	1085.50	Joback Method
cpg	1382.31	J/mol×K	1119.72	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=U308403&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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