

Benzamide, N,N-diundecyl-4-fluoro-

Inchi:	InChI=1S/C29H50FNO/c1-3-5-7-9-11-13-15-17-19-25-31(29(32)27-21-23-28(30)24-22-2
InchiKey:	NTRPYFGRHAXDPR-UHFFFAOYSA-N
Formula:	C29H50FNO
SMILES:	CCCCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	447.71

Physical Properties

Property code	Value	Unit	Source
gf	83.13	kJ/mol	Joback Method
hf	-657.99	kJ/mol	Joback Method
hfus	72.22	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-10.32		Crippen Method
logp	9.329		Crippen Method
mvol	409.030	ml/mol	McGowan Method
pc	742.45	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	960.16	K	Joback Method
tc	1179.28	K	Joback Method
tf	538.52	K	Joback Method
vc	1.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.18	J/molxK	960.16	Joback Method
cpg	1426.10	J/molxK	996.68	Joback Method
cpg	1446.61	J/molxK	1033.20	Joback Method
cpg	1465.83	J/molxK	1069.72	Joback Method
cpg	1483.86	J/molxK	1106.24	Joback Method
cpg	1500.81	J/molxK	1142.76	Joback Method
cpg	1516.78	J/molxK	1179.28	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U308313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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