

Benzamide, N,N-diundecyl-2,6-difluoro-

Inchi:	InChI=1S/C29H49F2NO/c1-3-5-7-9-11-13-15-17-19-24-32(25-20-18-16-14-12-10-8-6-4-2
InchiKey:	SXGQWRMFHAOUHF-UHFFFAOYSA-N
Formula:	C29H49F2NO
SMILES:	CCCCCCCCCCCCN(CCCCCCCCCCCC)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	465.70

Physical Properties

Property code	Value	Unit	Source
gf	-121.31	kJ/mol	Joback Method
hf	-865.57	kJ/mol	Joback Method
hfus	74.91	kJ/mol	Joback Method
hvap	90.90	kJ/mol	Joback Method
log10ws	-10.65		Crippen Method
logp	9.469		Crippen Method
mcvol	410.800	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	3131.00		NIST Webbook
tb	964.41	K	Joback Method
tc	1187.49	K	Joback Method
tf	551.63	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.98	J/mol×K	964.41	Joback Method
cpg	1432.96	J/mol×K	1001.59	Joback Method
cpg	1453.48	J/mol×K	1038.77	Joback Method
cpg	1472.64	J/mol×K	1075.95	Joback Method
cpg	1490.56	J/mol×K	1113.13	Joback Method
cpg	1507.34	J/mol×K	1150.31	Joback Method
cpg	1523.09	J/mol×K	1187.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U308673&Units=SI

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
hvac:	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

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