Benzamide, 2,5-difluoro-N-decyl-

Inchi: InChI=1S/C17H25F2NO/c1-2-3-4-5-6-7-8-9-12-20-17(21)15-13-14(18)10-11-16(15)19/h1
InchiKey: RGZYIHACEOEIJV-UHFFFAOYSA-N
Formula: C17H25F2NO
SMILES: CCCCCCCCCCNC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 297.38

Physical Properties

Property code	Value	Unit	Source
gf	-243.74	kJ/mol	Joback Method
hf	-631.95	kJ/mol	Joback Method
hfus	45.91	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.835		Crippen Method
mcvol	241.720	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	727.58	K	Joback Method
tc	913.02	K	Joback Method
tf	436.58	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.96	J/mol×K	727.58	Joback Method
cpg	715.74	J/mol×K	758.49	Joback Method
cpg	730.67	J/mol×K	789.39	Joback Method
cpg	744.75	J/mol×K	820.30	Joback Method
cpg	758.04	J/mol×K	851.20	Joback Method
cpg	770.56	J/mol×K	882.11	Joback Method
cpg	782.34	J/mol×K	913.02	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=U407592&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
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