

Cyclobutanecarboxamide, N-(4-fluorophenyl)-

Inchi:

lnchl=1S/C11H12FNO/c12-9-4-6-10(7-5-9)13-11(14)8-2-1-3-8/h4-8H,1-3H2,(H,13,14)

InchiKey:

REXMGRLJBVJXHN-UHFFFAOYSA-N

Formula:

C11H12FNO

SMILES:

O=C(Nc1ccc(F)cc1)C1CCC1

Mol. weight [g/mol]:

193.22

Physical Properties

Property code	Value	Unit	Source
gf	-41.17	kJ/mol	Joback Method
hf	-233.89	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.564		Crippen Method
mcvol	144.550	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	597.06	K	Joback Method
tc	821.69	K	Joback Method
tf	370.27	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.27	J/mol×K	597.06	Joback Method
cpg	380.28	J/mol×K	634.50	Joback Method
cpg	394.22	J/mol×K	671.94	Joback Method
cpg	407.14	J/mol×K	709.37	Joback Method
cpg	419.11	J/mol×K	746.81	Joback Method
cpg	430.18	J/mol×K	784.25	Joback Method
cpg	440.43	J/mol×K	821.69	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=U307046&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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