

4-Phenyl-4-chromancarboxamide

Inchi:	InChI=1S/C16H15NO2/c17-15(18)16(12-6-2-1-3-7-12)10-11-19-14-9-5-4-8-13(14)16/h1-15
InchiKey:	GJFSBFVZMHGUAV-UHFFFAOYSA-N
Formula:	C16H15NO2
SMILES:	NC(=O)C1(c2ccccc2)CCOc2ccccc21
Mol. weight [g/mol]:	253.30
CAS:	92962-91-9

Physical Properties

Property code	Value	Unit	Source
gf	193.60	kJ/mol	Joback Method
hf	-40.89	kJ/mol	Joback Method
hfus	29.40	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.240		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	788.42	K	Joback Method
tc	1059.45	K	Joback Method
tf	533.52	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.81	J/molxK	788.42	Joback Method
cpg	581.01	J/molxK	833.59	Joback Method
cpg	596.63	J/molxK	878.76	Joback Method
cpg	611.97	J/molxK	923.94	Joback Method
cpg	627.35	J/molxK	969.11	Joback Method
cpg	643.08	J/molxK	1014.28	Joback Method
cpg	659.48	J/molxK	1059.45	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=C92962919&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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