E-Isocroweacin

Inchi: InChI=1S/C11H12O3/c1-3-4-8-5-6-9-11(10(8)12-2)14-7-13-9/h3-6H,7H2,1-2H3/b4-3+
InchiKey: KLOOULZVSJNLAD-ONEGZZNKSA-N
Formula: C11H12O3
SMILES: CC=Cc1ccc2c(c1OC)OCO2
Mol. weight [g/mol]: 192.21
CAS: 194609-21-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.30	kJ/mol	Joback Method
hf	-254.11	kJ/mol	Joback Method
hfus	31.53	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.457		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1564.00		NIST Webbook
tb	584.59	K	Joback Method
tc	810.09	K	Joback Method
tf	370.18	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.19	J/mol×K	584.59	Joback Method
cpg	408.79	J/mol×K	772.51	Joback Method
cpg	398.55	J/mol×K	734.92	Joback Method
cpg	387.63	J/mol×K	697.34	Joback Method
cpg	375.97	J/mol×K	659.76	Joback Method
cpg	363.50	J/mol×K	622.17	Joback Method
cpg	418.39	J/mol×K	810.09	Joback Method
dvisc	0.0002949	Pa×s	584.59	Joback Method

dvisc	0.0003489	Pa×s	548.85	Joback Method
dvisc	0.0004226	Pa×s	513.12	Joback Method
dvisc	0.0005267	Pa×s	477.38	Joback Method
dvisc	0.0006803	Pa×s	441.65	Joback Method
dvisc	0.0009192	Pa×s	405.91	Joback Method
dvisc	0.0013163	Pa×s	370.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C194609217&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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