R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinoprop (desmethylene-desamino-oxo-), diethylated

InChI: InChI=1S/C13H16O4/c1-4-16-11-7-6-10(13(15)9(3)14)8-12(11)17-5-2/h6-8H,4-5H2,1-3H

InChIKey: HNGITVMKHKWGFD-UHFFFAOYSA-N

Formula: C13H16O4

SMILES: CCOc1ccc(C(=O)C(C)=O)cc1OCC

Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	-316.11	kJ/mol	Joback Method
hf	-587.66	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.256		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	686.06	K	Joback Method
tc	895.59	K	Joback Method
tf	432.05	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.62	J/mol×K	686.06	Joback Method
cpg	500.39	J/mol×K	720.98	Joback Method
cpg	513.32	J/mol×K	755.90	Joback Method
cpg	525.43	J/mol×K	790.82	Joback Method
cpg	536.70	J/mol×K	825.74	Joback Method
cpg	547.14	J/mol×K	860.66	Joback Method
cpg	556.74	J/mol×K	895.59	Joback Method
dvisc	0.0008784	Pa×s	432.05	Joback Method

dvisc	0.0005574	Pa×s	474.38	Joback Method
dvisc	0.0003810	Pa×s	516.72	Joback Method
dvisc	0.0002760	Pa×s	559.06	Joback Method
dvisc	0.0002091	Pa×s	601.39	Joback Method
dvisc	0.0001644	Pa×s	643.73	Joback Method
dvisc	0.0001331	Pa×s	686.06	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=R290714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/62-140-7/R-S-3-4-methylenedioxy-alpha-pyrrolidinopropiophenone-M-desmethylene-de
Generated by Cheméo on 2024-04-19 17:02:55.003951144 +0000 UTC m=+15835423.924528545.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.