Schkuhrianol Isomer

Inchi: InChI=1S/C29H50O6/c1-5-6-7-11-15-23(2)16-12-9-8-10-13-18-25(30)22-28(32)35-19-14
InchiKey: YVAXZNKKSLAKDG-UHFFFAOYSA-N
Formula: C29H50O6
SMILES: CCCCCCC(C)CCCCCCCC(O)CC(=O)OCCCc1cc(O)c(OC)c(OC)c1
Mol. weight [g/mol]: 494.70

Physical Properties

Property code	Value	Unit	Source
gf	-453.79	kJ/mol	Joback Method
hf	-1277.64	kJ/mol	Joback Method
hfus	72.12	kJ/mol	Joback Method
hvap	126.64	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.973		Crippen Method
mcvol	426.630	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	3722.40		NIST Webbook
rinpol	3722.40		NIST Webbook
tb	1192.61	K	Joback Method
tc	1513.12	K	Joback Method
tf	727.21	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1573.08	J/mol×K	1192.61	Joback Method
cpg	1659.29	J/mol×K	1459.70	Joback Method
cpg	1645.06	J/mol×K	1406.29	Joback Method
cpg	1629.58	J/mol×K	1352.87	Joback Method
cpg	1612.59	J/mol×K	1299.45	Joback Method
cpg	1593.84	J/mol×K	1246.03	Joback Method
cpg	1672.53	J/mol×K	1513.12	Joback Method
dvisc	2.0533134e-08	Pa×s	1192.61	Joback Method

dvisc	3.2537688e-08	Pa×s	1115.04	Joback Method
dvisc	5.5234925e-08	Pa×s	1037.48	Joback Method
dvisc	0.0000001	Pa×s	959.91	Joback Method
dvisc	0.0000002	Pa×s	882.34	Joback Method
dvisc	0.0000005	Pa×s	804.78	Joback Method
dvisc	0.0000014	Pa×s	727.21	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=U414677&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