o-Anisic acid, 6-pentadecyl ester

Inchi: InChI=1S/C23H38O3/c1-4-6-8-9-10-11-13-17-20(16-12-7-5-2)26-23(24)21-18-14-15-19-2
InchiKey: GMNWOPKXEHFSDT-UHFFFAOYSA-N
Formula: C23H38O3
SMILES: CCCCCCCCCC(CCCCC)OC(=O)c1ccccc1OC
Mol. weight [g/mol]: 362.55

Physical Properties

Property code	Value	Unit	Source
gf	-95.80	kJ/mol	Joback Method
hf	-675.29	kJ/mol	Joback Method
hfus	49.43	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.942		Crippen Method
mcvol	324.480	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2477.00		NIST Webbook
tb	855.57	K	Joback Method
tc	1052.74	K	Joback Method
tf	467.30	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.10	J/mol×K	855.57	Joback Method
cpg	1056.72	J/mol×K	888.43	Joback Method
cpg	1074.10	J/mol×K	921.29	Joback Method
cpg	1090.28	J/mol×K	954.15	Joback Method
cpg	1105.30	J/mol×K	987.01	Joback Method
cpg	1119.17	J/mol×K	1019.88	Joback Method
cpg	1131.93	J/mol×K	1052.74	Joback Method
dvisc	0.0006224	Pa×s	467.30	Joback Method
dvisc	0.0002861	Pa×s	532.01	Joback Method

dvisc	0.0001556	Pa×s	596.72	Joback Method
dvisc	0.0000954	Pa×s	661.43	Joback Method
dvisc	0.0000638	Pa×s	726.15	Joback Method
dvisc	0.0000456	Pa×s	790.86	Joback Method
dvisc	0.0000342	Pa×s	855.57	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=U299768&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