o-Anisic acid, heptadecyl ester

Inchi: InChI=1S/C25H42O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-28-25(26)23-20-17-1
InchiKey: CDHBRALYVRZRGF-UHFFFAOYSA-N
Formula: C25H42O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 390.60

Physical Properties

Property code	Value	Unit	Source
gf	-76.52	kJ/mol	Joback Method
hf	-711.29	kJ/mol	Joback Method
hfus	58.13	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.723		Crippen Method
mcvol	352.660	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
tb	901.77	K	Joback Method
tc	1104.50	K	Joback Method
tf	504.84	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.73	J/mol×K	901.77	Joback Method
cpg	1244.18	J/mol×K	1070.71	Joback Method
cpg	1230.22	J/mol×K	1036.92	Joback Method
cpg	1215.03	J/mol×K	1003.14	Joback Method
cpg	1198.58	J/mol×K	969.35	Joback Method
cpg	1180.82	J/mol×K	935.56	Joback Method
cpg	1256.96	J/mol×K	1104.50	Joback Method
dvisc	0.0000280	Pa×s	901.77	Joback Method

dvisc	0.0000369	Pa×s	835.61	Joback Method
dvisc	0.0000509	Pa×s	769.46	Joback Method
dvisc	0.0000747	Pa×s	703.30	Joback Method
dvisc	0.0001187	Pa×s	637.15	Joback Method
dvisc	0.0002100	Pa×s	571.00	Joback Method
dvisc	0.0004314	Pa×s	504.84	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=U299954&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
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