p-anisic acid, heptadecyl ester

Inchi: InChI=1S/C25H42O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-28-25(26)23-18-20-2
InchiKey: LNFOOKZBMMGPBM-UHFFFAOYSA-N
Formula: C25H42O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 390.61

Physical Properties

Property code	Value	Unit	Source
af	1.1740		Cheméo Relay (1.0)
hf	-760.54	kJ/mol	Cheméo Relay (1.0)
hfus	58.13	kJ/mol	Joback Method
hvap	125.71	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-7.96		Cheméo Relay (1.0)
logp	7.723		Crippen Method
mcvol	352.660	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinpol	2759.70		NIST Webbook
tb	670.96	K	Cheméo Relay (1.0)
tc	865.61	K	Cheméo Relay (1.0)
tf	328.49	K	Cheméo Relay (1.0)
vc	1.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.73	J/mol×K	901.77	Joback Method
cpg	1256.96	J/mol×K	1104.50	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
dvisc	0.0000747	Pa×s	703.30	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	0.0004314	Pa×s	504.84	Joback Method
dvisc	0.0001187	Pa×s	637.15	Joback Method
dvisc	0.0002100	Pa×s	571.00	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292463&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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