

o-Anisic acid, 2-pentadecyl ester

Inchi:	InChI=1S/C23H38O3/c1-4-5-6-7-8-9-10-11-12-13-14-17-20(2)26-23(24)21-18-15-16-19-2
InchiKey:	ACNRNCIIJZJUAX-UHFFFAOYSA-N
Formula:	C23H38O3
SMILES:	CCCCCCCCCCCCC(C)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
mvol	324.480	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	855.57	K	Joback Method
tc	1052.74	K	Joback Method
tf	467.30	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.10	J/molxK	855.57	Joback Method
cpg	1056.72	J/molxK	888.43	Joback Method
cpg	1074.10	J/molxK	921.29	Joback Method
cpg	1090.28	J/molxK	954.15	Joback Method
cpg	1105.30	J/molxK	987.01	Joback Method
cpg	1119.17	J/molxK	1019.88	Joback Method
cpg	1131.93	J/molxK	1052.74	Joback Method
dvisc	0.0006224	Paxs	467.30	Joback Method

dvisc	0.0002861	Paxs	532.01	Joback Method
dvisc	0.0001556	Paxs	596.72	Joback Method
dvisc	0.0000954	Paxs	661.43	Joback Method
dvisc	0.0000638	Paxs	726.15	Joback Method
dvisc	0.0000456	Paxs	790.86	Joback Method
dvisc	0.0000342	Paxs	855.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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