

o-Anisic acid, 4-hexadecyl ester

Inchi:	InChI=1S/C24H40O3/c1-4-6-7-8-9-10-11-12-13-14-18-21(17-5-2)27-24(25)22-19-15-16-2
InchiKey:	QXVJJCDERFZMGO-UHFFFAOYSA-N
Formula:	C24H40O3
SMILES:	CCCCCCCCCCCC(CCC)OC(=O)c1ccccc1OC
Mol. weight [g/mol]:	376.57

Physical Properties

Property code	Value	Unit	Source
gf	-87.38	kJ/mol	Joback Method
hf	-695.93	kJ/mol	Joback Method
hfus	52.02	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.332		Crippen Method
mcvol	338.570	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	878.45	K	Joback Method
tc	1078.15	K	Joback Method
tf	478.57	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.82	J/molxK	878.45	Joback Method
cpg	1118.67	J/molxK	911.73	Joback Method
cpg	1136.23	J/molxK	945.02	Joback Method
cpg	1152.53	J/molxK	978.30	Joback Method
cpg	1167.62	J/molxK	1011.59	Joback Method
cpg	1181.51	J/molxK	1044.87	Joback Method
cpg	1194.26	J/molxK	1078.15	Joback Method
dvisc	0.0005549	Paxs	478.57	Joback Method

dvisc	0.0002526	Paxs	545.22	Joback Method
dvisc	0.0001365	Paxs	611.86	Joback Method
dvisc	0.0000833	Paxs	678.51	Joback Method
dvisc	0.0000555	Paxs	745.16	Joback Method
dvisc	0.0000395	Paxs	811.80	Joback Method
dvisc	0.0000296	Paxs	878.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299953&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

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
mccvol:	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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