

o-Anisic acid, 4-tetradecyl ester

Inchi: InChI=1S/C22H36O3/c1-4-6-7-8-9-10-11-12-16-19(15-5-2)25-22(23)20-17-13-14-18-21(2)
InchiKey: BXADSDIUNMZOGX-UHFFFAOYSA-N
Formula: C22H36O3
SMILES: CCCCCCCCCC(CCC)OC(=O)c1ccccc1OC
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
gf	-104.22	kJ/mol	Joback Method
hf	-654.65	kJ/mol	Joback Method
hfus	46.84	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.551		Crippen Method
mvol	310.390	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinpol	2403.00		NIST Webbook
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tb	832.69	K	Joback Method
tc	1028.10	K	Joback Method
tf	456.03	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.05	J/molxK	832.69	Joback Method
cpg	1057.51	J/molxK	995.53	Joback Method
cpg	1043.67	J/molxK	962.96	Joback Method
cpg	1028.73	J/molxK	930.39	Joback Method
cpg	1012.66	J/molxK	897.83	Joback Method
cpg	995.45	J/molxK	865.26	Joback Method
cpg	1070.27	J/molxK	1028.10	Joback Method
dvisc	0.0000395	Paxs	832.69	Joback Method

dvisc	0.0000524	Paxs	769.91	Joback Method
dvisc	0.0000731	Paxs	707.14	Joback Method
dvisc	0.0001089	Paxs	644.36	Joback Method
dvisc	0.0001769	Paxs	581.58	Joback Method
dvisc	0.0003228	Paxs	518.81	Joback Method
dvisc	0.0006955	Paxs	456.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299763&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

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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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