

o-Anisic acid, 4-tridecyl ester

Inchi:	InChI=1S/C21H34O3/c1-4-6-7-8-9-10-11-15-18(14-5-2)24-21(22)19-16-12-13-17-20(19)2
InchiKey:	NMBUPNBVEJSGFJ-UHFFFAOYSA-N
Formula:	C21H34O3
SMILES:	CCCCCCCCC(CCC)OC(=O)c1ccccc1OC
Mol. weight [g/mol]:	334.49

Physical Properties

Property code	Value	Unit	Source
gf	-112.64	kJ/mol	Joback Method
hf	-634.01	kJ/mol	Joback Method
hfus	44.25	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.161		Crippen Method
mcvol	296.300	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	809.81	K	Joback Method
tc	1004.18	K	Joback Method
tf	444.76	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.73	J/molxK	809.81	Joback Method
cpg	996.56	J/molxK	971.78	Joback Method
cpg	982.77	J/molxK	939.39	Joback Method
cpg	967.92	J/molxK	906.99	Joback Method
cpg	951.98	J/molxK	874.60	Joback Method
cpg	934.92	J/molxK	842.20	Joback Method
cpg	1009.32	J/molxK	1004.18	Joback Method
dvisc	0.0000454	Paxs	809.81	Joback Method

dvisc	0.0000601	Paxs	748.97	Joback Method
dvisc	0.0000836	Paxs	688.13	Joback Method
dvisc	0.0001241	Paxs	627.28	Joback Method
dvisc	0.0002003	Paxs	566.44	Joback Method
dvisc	0.0003630	Paxs	505.60	Joback Method
dvisc	0.0007740	Paxs	444.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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