

o-Toluic acid, 3-pentadecyl ester

Other names:	o-Toluylic acid, 3-pentadecyl ester
Inchi:	InChI=1S/C23H38O2/c1-4-6-7-8-9-10-11-12-13-14-18-21(5-2)25-23(24)22-19-16-15-17-2
InchiKey:	WUOZPZGNWDBHIV-UHFFFAOYSA-N
Formula:	C23H38O2
SMILES:	CCCCCCCCCCCCC(CC)OC(=O)c1ccccc1C
Mol. weight [g/mol]:	346.55

Physical Properties

Property code	Value	Unit	Source
gf	9.20	kJ/mol	Joback Method
hf	-543.07	kJ/mol	Joback Method
hfus	48.24	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.241		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	833.15	K	Joback Method
tc	1028.23	K	Joback Method
tf	445.07	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.47	J/molxK	833.15	Joback Method
cpg	1025.53	J/molxK	865.66	Joback Method
cpg	1043.42	J/molxK	898.18	Joback Method
cpg	1060.20	J/molxK	930.69	Joback Method
cpg	1075.90	J/molxK	963.20	Joback Method
cpg	1090.56	J/molxK	995.71	Joback Method
cpg	1104.22	J/molxK	1028.23	Joback Method

dvisc	0.0009154	Paxs	445.07	Joback Method
dvisc	0.0004045	Paxs	509.75	Joback Method
dvisc	0.0002149	Paxs	574.43	Joback Method
dvisc	0.0001297	Paxs	639.11	Joback Method
dvisc	0.0000859	Paxs	703.79	Joback Method
dvisc	0.0000610	Paxs	768.47	Joback Method
dvisc	0.0000457	Paxs	833.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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