

o-Toluic acid, heptadecyl ester

Other names:	o-toluylic acid, heptadecyl ester
Inchi:	InChI=1S/C25H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-27-25(26)24-21-18-
InchiKey:	GQELEXWZTMWWJM-UHFFFAOYSA-N
Formula:	C25H42O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	374.60

Physical Properties

Property code	Value	Unit	Source
gf	28.48	kJ/mol	Joback Method
hf	-579.07	kJ/mol	Joback Method
hfus	56.94	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.023		Crippen Method
mvol	346.790	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2725.40		NIST Webbook
tb	879.35	K	Joback Method
tc	1078.25	K	Joback Method
tf	482.61	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.80	J/molxK	879.35	Joback Method
cpg	1149.32	J/molxK	912.50	Joback Method
cpg	1167.61	J/molxK	945.65	Joback Method
cpg	1184.71	J/molxK	978.80	Joback Method
cpg	1200.69	J/molxK	1011.95	Joback Method
cpg	1215.57	J/molxK	1045.10	Joback Method
cpg	1229.43	J/molxK	1078.25	Joback Method
dvisc	0.0006292	Paxs	482.61	Joback Method

dvisc	0.0002964	Paxs	548.73	Joback Method
dvisc	0.0001641	Paxs	614.86	Joback Method
dvisc	0.0001020	Paxs	680.98	Joback Method
dvisc	0.0000689	Paxs	747.10	Joback Method
dvisc	0.0000496	Paxs	813.23	Joback Method
dvisc	0.0000376	Paxs	879.35	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=U292231&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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