

o-Toluic acid, octadecyl ester

Other names:	o-Toluylic acid, octadecyl ester
Inchi:	InChI=1S/C26H44O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-28-26(27)25-22-1
InchiKey:	DDBNDPFMAYKYRG-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	388.63

Physical Properties

Property code	Value	Unit	Source
gf	36.90	kJ/mol	Joback Method
hf	-599.71	kJ/mol	Joback Method
hfus	59.53	kJ/mol	Joback Method
hvap	85.56	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.413		Crippen Method
mvol	360.880	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinpol	2815.80		NIST Webbook
tb	902.23	K	Joback Method
tc	1104.96	K	Joback Method
tf	493.88	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.67	J/molxK	902.23	Joback Method
cpg	1212.53	J/molxK	936.02	Joback Method
cpg	1231.10	J/molxK	969.81	Joback Method
cpg	1248.44	J/molxK	1003.60	Joback Method
cpg	1264.59	J/molxK	1037.39	Joback Method
cpg	1279.61	J/molxK	1071.18	Joback Method
cpg	1293.56	J/molxK	1104.96	Joback Method
dvisc	0.0005613	Paxs	493.88	Joback Method

dvisc	0.0002619	Paxs	561.94	Joback Method
dvisc	0.0001441	Paxs	630.00	Joback Method
dvisc	0.0000890	Paxs	698.05	Joback Method
dvisc	0.0000599	Paxs	766.11	Joback Method
dvisc	0.0000430	Paxs	834.17	Joback Method
dvisc	0.0000325	Paxs	902.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292386&Units=SI

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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