

1,1,2-Tritolyethane

Inchi:	InChI=1S/C23H24/c1-17-4-10-20(11-5-17)16-23(21-12-6-18(2)7-13-21)22-14-8-19(3)9-1
InchiKey:	UELJFQQBQVFDMT-UHFFFAOYSA-N
Formula:	C23H24
SMILES:	Cc1ccc(CC(c2ccc(C)cc2)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	300.44
CAS:	27497-47-8

Physical Properties

Property code	Value	Unit	Source
chs	-12497.10 ± 3.00	kJ/mol	NIST Webbook
gf	448.68	kJ/mol	Joback Method
hf	151.85	kJ/mol	Joback Method
hfus	32.76	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.986		Crippen Method
mvol	263.650	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
tb	820.18	K	Joback Method
tc	1067.81	K	Joback Method
tf	450.79	K	Joback Method
vc	0.994	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.10	J/molxK	820.18	Joback Method
cpg	789.69	J/molxK	861.45	Joback Method
cpg	806.78	J/molxK	902.72	Joback Method
cpg	822.48	J/molxK	943.99	Joback Method
cpg	836.90	J/molxK	985.26	Joback Method
cpg	850.15	J/molxK	1026.54	Joback Method
cpg	862.34	J/molxK	1067.81	Joback Method
dvisc	0.0007773	Paxs	450.79	Joback Method

dvisc	0.0004034	Paxs	512.36	Joback Method
dvisc	0.0002410	Paxs	573.92	Joback Method
dvisc	0.0001591	Paxs	635.49	Joback Method
dvisc	0.0001130	Paxs	697.05	Joback Method
dvisc	0.0000849	Paxs	758.62	Joback Method
dvisc	0.0000665	Paxs	820.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27497478&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/10-441-0/1-1-2-Tritolyethane.pdf>

Generated by Cheméo on 2024-04-17 02:54:18.619475269 +0000 UTC m=+15611707.540052589.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.