

Ether, «alpha»,«alpha»-dimethylbenzyl propyl

Other names:	«alpha»,«alpha»-Dimethylbenzyl propyl ether Benzene, (1-methyl-1-propoxyethyl)- (1-methyl-1-propoxyethyl)benzene Propyl cumyl ether
Inchi:	InChI=1S/C12H18O/c1-4-10-13-12(2,3)11-8-6-5-7-9-11/h5-9H,4,10H2,1-3H3
InchiKey:	PLWOFDYJSDGEAT-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCOC(C)(C)c1ccccc1
Mol. weight [g/mol]:	178.27
CAS:	24142-77-6

Physical Properties

Property code	Value	Unit	Source
gf	60.41	kJ/mol	Joback Method
hf	-195.45	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	59.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.20		Crippen Method
logp	3.348		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	519.83	K	Joback Method
tc	730.01	K	Joback Method
tf	276.07	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.77	J/mol×K	730.01	Joback Method
cpg	374.88	J/mol×K	519.83	Joback Method
cpg	392.52	J/mol×K	554.86	Joback Method
cpg	409.11	J/mol×K	589.89	Joback Method
cpg	424.68	J/mol×K	624.92	Joback Method

cpg	439.28	J/mol×K	659.95	Joback Method
cpg	452.97	J/mol×K	694.98	Joback Method
dvisc	0.0001636	Pa×s	519.83	Joback Method
dvisc	0.0037027	Pa×s	276.07	Joback Method
dvisc	0.0015773	Pa×s	316.70	Joback Method
dvisc	0.0008158	Pa×s	357.32	Joback Method
dvisc	0.0004828	Pa×s	397.95	Joback Method
dvisc	0.0003148	Pa×s	438.58	Joback Method
dvisc	0.0002208	Pa×s	479.20	Joback Method
hvapt	59.10 ± 0.20	kJ/mol	301.50	NIST Webbook

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=C24142776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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