

Mesityl-acetomesitylene

Inchi:	InChI=1S/C20H24O/c1-12-7-14(3)18(15(4)8-12)11-19(21)20-16(5)9-13(2)10-17(20)6/h7-
InchiKey:	VEQCXWMGUSPDQV-UHFFFAOYSA-N
Formula:	C20H24O
SMILES:	Cc1cc(C)c(CC(=O)c2c(C)cc(C)cc2C)c(C)c1
Mol. weight [g/mol]:	280.40
CAS:	5796-78-1

Physical Properties

Property code	Value	Unit	Source
gf	155.64	kJ/mol	Joback Method
hf	-164.47	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.963		Crippen Method
mcvol	246.710	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
tb	794.11	K	Joback Method
tc	1019.07	K	Joback Method
tf	493.05	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.71	J/mol×K	794.11	Joback Method
cpg	779.08	J/mol×K	981.58	Joback Method
cpg	766.55	J/mol×K	944.08	Joback Method
cpg	752.98	J/mol×K	906.59	Joback Method
cpg	738.35	J/mol×K	869.10	Joback Method
cpg	722.60	J/mol×K	831.60	Joback Method
cpg	790.62	J/mol×K	1019.07	Joback Method
dvisc	0.0001040	Pa×s	794.11	Joback Method
dvisc	0.0001253	Pa×s	743.93	Joback Method

dvisc	0.0001552	Pa×s	693.76	Joback Method
dvisc	0.0001987	Pa×s	643.58	Joback Method
dvisc	0.0002653	Pa×s	593.40	Joback Method
dvisc	0.0003735	Pa×s	543.23	Joback Method
dvisc	0.0005640	Pa×s	493.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5796781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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