

3-Ethyl-3-methylglutaric anhydride

Other names:	«beta»-Methyl-«beta»-ethylglutaric anhydride 2H-Pyran-2,6(3H)-dione, 4-ethyl-dihydro-4-methyl-
Inchi:	InChI=1S/C8H12O3/c1-3-8(2)4-6(9)11-7(10)5-8/h3-5H2,1-2H3
InchiKey:	VSVZSLYJGKSCBI-UHFFFAOYSA-N
Formula:	C8H12O3
SMILES:	CCC1(C)CC(=O)OC(=O)C1
Mol. weight [g/mol]:	156.18
CAS:	6970-57-6

Physical Properties

Property code	Value	Unit	Source
gf	-295.86	kJ/mol	Joback Method
hf	-546.29	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	45.68	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.266		Crippen Method
mvol	121.730	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	564.82	K	Joback Method
tc	809.13	K	Joback Method
tf	374.21	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.05	J/mol×K	564.82	Joback Method
cpg	320.82	J/mol×K	605.54	Joback Method
cpg	335.80	J/mol×K	646.26	Joback Method
cpg	350.05	J/mol×K	686.98	Joback Method
cpg	363.64	J/mol×K	727.69	Joback Method
cpg	376.63	J/mol×K	768.41	Joback Method
cpg	389.09	J/mol×K	809.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	2.70	NIST Webbook

Sources

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=C6970576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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