2,4,4-TRIMETHYLBUT-2-ENOLIDE

Other names: 2,4,4-Trimethyl-2-butenolide
3,5,5-trimethyl-2(5H)-furanone
Inchi: InChI=1S/C7H10O2/c1-5-4-7(2,3)9-6(5)8/h4H,1-3H3
InchiKey: OAVLYQLCBORARJ-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1=CC(C)(C)OC1=O
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
hfus	9.84	kJ/mol	Joback Method
logp	1.268		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
tf	293.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.58	J/mol×K	473.99	Joback Method
cpg	232.11	J/mol×K	511.86	Joback Method
cpg	243.87	J/mol×K	549.73	Joback Method
cpg	254.94	J/mol×K	587.60	Joback Method
cpg	265.41	J/mol×K	625.47	Joback Method
cpg	275.38	J/mol×K	663.34	Joback Method
cpg	284.92	J/mol×K	701.21	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50598500&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tf:	Normal melting (fusion) point