4,6-Eudesmadiene-3,8-dione

Inchi: InChI=1S/C15H20O2/c1-9(2)11-7-12-10(3)13(16)5-6-15(12,4)8-14(11)17/h7,9H,5-6,8H2,
InchiKey: LLOYUVLMNHQEFN-HNNXBMFYSA-N
Formula: C15H20O2
SMILES: CC1=C2C=C(C(C)C)C(=O)CC2(C)CCC1=O
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	-65.85	kJ/mol	Joback Method
hf	-395.92	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.227		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1833.00		NIST Webbook
ripol	2492.00		NIST Webbook
tb	726.53	K	Joback Method
tc	974.95	K	Joback Method
tf	469.27	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.21	J/mol×K	726.53	Joback Method
cpg	590.99	J/mol×K	767.93	Joback Method
cpg	609.82	J/mol×K	809.34	Joback Method
cpg	627.80	J/mol×K	850.74	Joback Method
cpg	645.07	J/mol×K	892.14	Joback Method
cpg	661.74	J/mol×K	933.55	Joback Method
cpg	677.92	J/mol×K	974.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321001&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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