Orcinyl di-tiglate

Inchi: InChI=1S/C17H20O4/c1-6-12(4)16(18)20-14-8-11(3)9-15(10-14)21-17(19)13(5)7-2/h6-10
InchiKey: OTIFHGKSAXGGTI-PWHKKFIBSA-N
Formula: C17H20O4
SMILES: CC=C(C)C(=O)Oc1cc(C)cc(OC(=O)C(C)=CC)c1
Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-139.09	kJ/mol	Joback Method
hf	-455.36	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.738		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
ripol	3128.00		NIST Webbook
ripol	3128.00		NIST Webbook
tb	785.66	K	Joback Method
tc	1004.27	K	Joback Method
tf	439.05	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.36	J/mol×K	785.66	Joback Method
cpg	667.00	J/mol×K	822.09	Joback Method
cpg	680.67	J/mol×K	858.53	Joback Method
cpg	693.38	J/mol×K	894.96	Joback Method
cpg	705.19	J/mol×K	931.40	Joback Method
cpg	716.13	J/mol×K	967.83	Joback Method
cpg	726.24	J/mol×K	1004.27	Joback Method

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=U383594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

https://www.chemeo.com/cid/90-469-2/Orcinyl-di-tiglate.pdf

Generated by Cheméo on 2024-10-12 02:46:03.589780021 +0000 UTC m=+3282026.226749269.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.