4,4'-DIMETHYLBENZOIC ANHYDRIDE

Inchi: InChI=1S/C16H14O3/c1-11-3-7-13(8-4-11)15(17)19-16(18)14-9-5-12(2)6-10-14/h3-10H,1
InchiKey: BJMLLSSSTGHJJE-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: Cc1ccc(C(=O)OC(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 254.29

Physical Properties

Property code	Value	Unit	Source
af	0.7127		Cheméo Relay (1.0)
chs	-7776.00 ± 7.90	kJ/mol	NIST Webbook
gf	-73.44	kJ/mol	Joback Method
hf	-399.99	kJ/mol	Cheméo Relay (1.0)
hfs	-521.00 ± 7.90	kJ/mol	NIST Webbook
hfus	28.89	kJ/mol	Joback Method
hvap	91.22	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-4.27		Cheméo Relay (1.0)
logp	3.301		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	629.84	K	Cheméo Relay (1.0)
tc	874.19	K	Cheméo Relay (1.0)
tf	365.25	K	Cheméo Relay (1.0)
vc	0.734	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.45	J/mol×K	758.96	Joback Method
cpg	597.96	J/mol×K	998.86	Joback Method
cpg	589.55	J/mol×K	958.87	Joback Method
cpg	580.13	J/mol×K	918.89	Joback Method
cpg	569.64	J/mol×K	878.91	Joback Method
cpg	558.06	J/mol×K	838.93	Joback Method

cpg	545.35	J/mol×K	798.94	Joback Method
dvisc	0.0002595	Pa×s	614.50	Joback Method
dvisc	0.0001235	Pa×s	758.96	Joback Method
dvisc	0.0001530	Pa×s	710.81	Joback Method
dvisc	0.0001955	Pa×s	662.66	Joback Method
dvisc	0.0008599	Pa×s	470.05	Joback Method
dvisc	0.0003615	Pa×s	566.35	Joback Method
dvisc	0.0005355	Pa×s	518.20	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=C13222850&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

af: Acentric Factor
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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