Dibenzoyl, 4-dimethylamino

Inchi: InChI=1S/C16H15NO2/c1-17(2)14-10-8-13(9-11-14)16(19)15(18)12-6-4-3-5-7-12/h3-11H
InchiKey: CRMRQULUOONHLY-UHFFFAOYSA-N
Formula: C16H15NO2
SMILES: CN(C)c1ccc(C(=O)C(=O)c2ccccc2)cc1
Mol. weight [g/mol]: 253.30

Physical Properties

Property code	Value	Unit	Source
gf	151.97	kJ/mol	Joback Method
hf	-69.61	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.818		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	744.00	K	Joback Method
tc	982.92	K	Joback Method
tf	467.77	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.27	J/mol×K	744.00	Joback Method
cpg	560.86	J/mol×K	783.82	Joback Method
cpg	574.22	J/mol×K	823.64	Joback Method
cpg	586.44	J/mol×K	863.46	Joback Method
cpg	597.58	J/mol×K	903.28	Joback Method
cpg	607.76	J/mol×K	943.10	Joback Method
cpg	617.03	J/mol×K	982.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121158&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

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

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