

1,3-Di-(2,4-dimethyl-benzoyl)-propane

Inchi:	InChI=1S/C21H24O2/c1-14-8-10-18(16(3)12-14)20(22)6-5-7-21(23)19-11-9-15(2)13-17(
InchiKey:	GWLPWMUYNCDPJK-UHFFFAOYSA-N
Formula:	C21H24O2
SMILES:	<chem>Cc1ccc(C(=O)CCCC(=O)c2ccc(C)cc2C)c(C)c1</chem>
Mol. weight [g/mol]:	308.41
CAS:	6280-01-9

Physical Properties

Property code	Value	Unit	Source
gf	54.40	kJ/mol	Joback Method
hf	-274.75	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.156		Crippen Method
mcvol	262.370	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
tb	860.90	K	Joback Method
tc	1087.39	K	Joback Method
tf	529.21	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.71	J/molxK	860.90	Joback Method
cpg	796.04	J/molxK	898.65	Joback Method
cpg	810.20	J/molxK	936.40	Joback Method
cpg	823.25	J/molxK	974.14	Joback Method
cpg	835.23	J/molxK	1011.89	Joback Method
cpg	846.20	J/molxK	1049.64	Joback Method
cpg	856.22	J/molxK	1087.39	Joback Method
dvisc	0.0006166	Paxs	529.21	Joback Method
dvisc	0.0003846	Paxs	584.49	Joback Method

dvisc	0.0002602	Paxs	639.77	Joback Method
dvisc	0.0001874	Paxs	695.06	Joback Method
dvisc	0.0001416	Paxs	750.34	Joback Method
dvisc	0.0001112	Paxs	805.62	Joback Method
dvisc	0.0000901	Paxs	860.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6280019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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