

Ethyl-a,a-dibenzylacetoacetate

Inchi:	InChI=1S/C20H22O3/c1-3-23-19(22)20(16(2)21,14-17-10-6-4-7-11-17)15-18-12-8-5-9-13
InchiKey:	GAEGCFQREIOAKQ-UHFFFAOYSA-N
Formula:	C20H22O3
SMILES:	CCOC(=O)C(Cc1ccccc1)(Cc1ccccc1)C(C)=O
Mol. weight [g/mol]:	310.39
CAS:	42597-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.66	kJ/mol	Joback Method
hf	-349.20	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.610		Crippen Method
mcvol	254.150	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
tb	837.29	K	Joback Method
tc	1071.18	K	Joback Method
tf	492.51	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.39	J/molxK	837.29	Joback Method
cpg	820.90	J/molxK	1032.20	Joback Method
cpg	810.17	J/molxK	993.22	Joback Method
cpg	798.45	J/molxK	954.24	Joback Method
cpg	785.65	J/molxK	915.25	Joback Method
cpg	771.66	J/molxK	876.27	Joback Method
cpg	830.74	J/molxK	1071.18	Joback Method
dvisc	0.0000581	Paxs	837.29	Joback Method
dvisc	0.0000764	Paxs	779.83	Joback Method

dvisc	0.0001050	Paxs	722.36	Joback Method
dvisc	0.0001525	Paxs	664.90	Joback Method
dvisc	0.0002375	Paxs	607.44	Joback Method
dvisc	0.0004059	Paxs	549.97	Joback Method
dvisc	0.0007861	Paxs	492.51	Joback Method

Sources

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=C42597262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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