1-(4-Benzylphenyl)-1-butanone

Inchi: InChI=1S/C17H18O/c1-2-6-17(18)16-11-9-15(10-12-16)13-14-7-4-3-5-8-14/h3-5,7-12H,2
InchiKey: CQGHAVUWNSCNMH-UHFFFAOYSA-N
Formula: C17H18O
SMILES: CCCC(=O)c1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]: 238.32
CAS: 17302-69-1

Physical Properties

Property code	Value	Unit	Source
gf	178.53	kJ/mol	Joback Method
hf	-45.20	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.260		Crippen Method
mcvol	204.440	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	700.57	K	Joback Method
tc	933.15	K	Joback Method
tf	396.64	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.35	J/mol×K	700.57	Joback Method
cpg	561.15	J/mol×K	739.33	Joback Method
cpg	576.71	J/mol×K	778.10	Joback Method
cpg	591.09	J/mol×K	816.86	Joback Method
cpg	604.36	J/mol×K	855.62	Joback Method
cpg	616.60	J/mol×K	894.39	Joback Method
cpg	627.89	J/mol×K	933.15	Joback Method
dvisc	0.0015064	Pa×s	396.64	Joback Method
dvisc	0.0008101	Pa×s	447.29	Joback Method

dvisc	0.0004942	Pa×s	497.95	Joback Method
dvisc	0.0003303	Pa×s	548.61	Joback Method
dvisc	0.0002363	Pa×s	599.26	Joback Method
dvisc	0.0001781	Pa×s	649.91	Joback Method
dvisc	0.0001399	Pa×s	700.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302691&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume