n-Butyl 4-oxo-4-(4-phenylphenyl)butanoate

Inchi: InChI=1S/C20H22O3/c1-2-3-15-23-20(22)14-13-19(21)18-11-9-17(10-12-18)16-7-5-4-6-8
InchiKey: WYFZCKWYWSPBDR-UHFFFAOYSA-N
Formula: C20H22O3
SMILES: CCCCOC(=O)CCC(=O)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 310.39

Physical Properties

Property code	Value	Unit	Source
gf	-30.13	kJ/mol	Joback Method
hf	-351.92	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	81.23	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.660		Crippen Method
mcvol	254.150	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2793.00		NIST Webbook
tb	845.50	K	Joback Method
tc	1070.55	K	Joback Method
tf	502.61	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.03	J/mol×K	845.50	Joback Method
cpg	768.88	J/mol×K	883.01	Joback Method
cpg	782.50	J/mol×K	920.52	Joback Method
cpg	794.96	J/mol×K	958.03	Joback Method
cpg	806.31	J/mol×K	995.54	Joback Method
cpg	816.62	J/mol×K	1033.04	Joback Method
cpg	825.92	J/mol×K	1070.55	Joback Method
dvisc	0.0007259	Pa×s	502.61	Joback Method
dvisc	0.0004090	Pa×s	559.76	Joback Method

dvisc	0.0002563	Pa×s	616.91	Joback Method
dvisc	0.0001739	Pa×s	674.06	Joback Method
dvisc	0.0001253	Pa×s	731.20	Joback Method
dvisc	0.0000947	Pa×s	788.35	Joback Method
dvisc	0.0000744	Pa×s	845.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372924&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume