4-Butylbenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C16H22O2/c1-4-5-6-14-7-9-15(10-8-14)16(17)18-12-11-13(2)3/h7-11H,4-6,12H
InchiKey: MXTDRGHCGUHVIH-UHFFFAOYSA-N
Formula: C16H22O2
SMILES: CCCCc1ccc(C(=O)OCC=C(C)C)cc1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	24.37	kJ/mol	Joback Method
hf	-285.88	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.152		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1924.40		NIST Webbook
tb	677.47	K	Joback Method
tc	883.60	K	Joback Method
tf	362.14	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.28	J/mol×K	677.47	Joback Method
cpg	594.03	J/mol×K	711.82	Joback Method
cpg	609.80	J/mol×K	746.18	Joback Method
cpg	624.63	J/mol×K	780.53	Joback Method
cpg	638.56	J/mol×K	814.89	Joback Method
cpg	651.64	J/mol×K	849.24	Joback Method
cpg	663.89	J/mol×K	883.60	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=U292520&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
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