Cyclohexanecarboxylic acid, 4-butyl-, 4-ethoxyphenyl ester, trans-

Other names: trans-4-Butylcyclohexanecarboxylic acid, 4-ethoxyphenyl ester
4-ethoxyphenyl trans-4-butylcyclohexanoate

Inchi: InChI=1S/C19H28O3/c1-3-5-6-15-7-9-16(10-8-15)19(20)22-18-13-11-17(12-14-18)21-4-2

InchiKey: JAYBMJPZPJBTQZ-WKILWMFISA-N

Formula: C19H28O3

SMILES: CCCCC1CCC(C(=O)Oc2ccc(OCC)cc2)CC1

Mol. weight [g/mol]: 304.42

CAS: 67589-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-110.30	kJ/mol	Joback Method
hf	-553.47	kJ/mol	Joback Method
hfus	35.50	kJ/mol	Joback Method
hvap	72.51	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.987		Crippen Method
mcvol	257.260	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
tb	779.37	K	Joback Method
tc	994.17	K	Joback Method
tf	440.36	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.87	J/mol×K	779.37	Joback Method
cpg	816.59	J/mol×K	815.17	Joback Method
cpg	834.86	J/mol×K	850.97	Joback Method
cpg	851.69	J/mol×K	886.77	Joback Method
cpg	867.12	J/mol×K	922.57	Joback Method
cpg	881.15	J/mol×K	958.37	Joback Method
cpg	893.81	J/mol×K	994.17	Joback Method

dvisc	0.0009556	Pa×s	440.36	Joback Method
dvisc	0.0005078	Pa×s	496.86	Joback Method
dvisc	0.0003070	Pa×s	553.36	Joback Method
dvisc	0.0002038	Pa×s	609.87	Joback Method
dvisc	0.0001450	Pa×s	666.37	Joback Method
dvisc	0.0001088	Pa×s	722.87	Joback Method
dvisc	0.0000851	Pa×s	779.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67589473&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