

4-Butylbenzoic acid, 4-hexadecyl ester

Inchi:	InChI=1S/C27H46O2/c1-4-7-9-10-11-12-13-14-15-16-19-26(17-6-3)29-27(28)25-22-20-2
InchiKey:	KKYOILIMTNHJLV-UHFFFAOYSA-N
Formula:	C27H46O2
SMILES:	CCCCCCCCCCCC(CCC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	402.65

Physical Properties

Property code	Value	Unit	Source
gf	42.88	kJ/mol	Joback Method
hf	-625.63	kJ/mol	Joback Method
hfus	58.60	kJ/mol	Joback Method
hvap	87.40	kJ/mol	Joback Method
log10ws	-9.74		Crippen Method
logp	8.666		Crippen Method
mvol	374.970	ml/mol	McGowan Method
pc	845.05	kPa	Joback Method
rinpol	2627.60		NIST Webbook
tb	924.67	K	Joback Method
tc	1132.09	K	Joback Method
tf	490.15	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.50	J/molxK	924.67	Joback Method
cpg	1344.44	J/molxK	1097.52	Joback Method
cpg	1329.35	J/molxK	1062.95	Joback Method
cpg	1313.07	J/molxK	1028.38	Joback Method
cpg	1295.54	J/molxK	993.81	Joback Method
cpg	1276.71	J/molxK	959.24	Joback Method
cpg	1358.40	J/molxK	1132.09	Joback Method
dvisc	0.0000256	Paxs	924.67	Joback Method
dvisc	0.0000345	Paxs	852.25	Joback Method

dvisc	0.0000491	Paxs	779.83	Joback Method
dvisc	0.0000751	Paxs	707.41	Joback Method
dvisc	0.0001267	Paxs	634.99	Joback Method
dvisc	0.0002444	Paxs	562.57	Joback Method
dvisc	0.0005724	Paxs	490.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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