

4-Butylbenzoic acid, 5-tridecyl ester

Inchi:	InChI=1S/C24H40O2/c1-4-7-10-11-12-13-16-23(15-9-6-3)26-24(25)22-19-17-21(18-20-2
InchiKey:	HDKNQOESLTENR-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCC(CCCC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
gf	17.62	kJ/mol	Joback Method
hf	-563.71	kJ/mol	Joback Method
hfus	50.83	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.495		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinsol	2498.00		NIST Webbook
tb	856.03	K	Joback Method
tc	1052.96	K	Joback Method
tf	456.34	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.02	J/molxK	856.03	Joback Method
cpg	1087.32	J/molxK	888.85	Joback Method
cpg	1105.41	J/molxK	921.67	Joback Method
cpg	1122.35	J/molxK	954.50	Joback Method
cpg	1138.18	J/molxK	987.32	Joback Method
cpg	1152.93	J/molxK	1020.14	Joback Method
cpg	1166.67	J/molxK	1052.96	Joback Method
dvisc	0.0008185	Paxs	456.34	Joback Method
dvisc	0.0003584	Paxs	522.95	Joback Method

dvisc	0.0001891	Paxs	589.57	Joback Method
dvisc	0.0001136	Paxs	656.18	Joback Method
dvisc	0.0000750	Paxs	722.80	Joback Method
dvisc	0.0000531	Paxs	789.41	Joback Method
dvisc	0.0000397	Paxs	856.03	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=U299939&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
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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