

4-Butylbenzoic acid, 4-pentadecyl ester

Inchi:	InChI=1S/C26H44O2/c1-4-7-9-10-11-12-13-14-15-18-25(16-6-3)28-26(27)24-21-19-23(2
InchiKey:	KMTISKGELRHBQX-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCC(CCC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	388.63

Physical Properties

Property code	Value	Unit	Source
gf	34.46	kJ/mol	Joback Method
hf	-604.99	kJ/mol	Joback Method
hfus	56.01	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	8.276		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	894.27	kPa	Joback Method
rinsol	2693.00		NIST Webbook
tb	901.79	K	Joback Method
tc	1104.83	K	Joback Method
tf	478.88	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.09	J/molxK	901.79	Joback Method
cpg	1279.91	J/molxK	1070.99	Joback Method
cpg	1264.94	J/molxK	1037.15	Joback Method
cpg	1248.82	J/molxK	1003.31	Joback Method
cpg	1231.52	J/molxK	969.47	Joback Method
cpg	1212.95	J/molxK	935.63	Joback Method
cpg	1293.79	J/molxK	1104.83	Joback Method
dvisc	0.0000297	Paxs	901.79	Joback Method
dvisc	0.0000399	Paxs	831.31	Joback Method

dvisc	0.0000567	Paxs	760.82	Joback Method
dvisc	0.0000865	Paxs	690.34	Joback Method
dvisc	0.0001452	Paxs	619.85	Joback Method
dvisc	0.0002785	Paxs	549.37	Joback Method
dvisc	0.0006471	Paxs	478.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299945&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
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
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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