

4-Butylbenzoic acid, 2-tetradecyl ester

Inchi:	InChI=1S/C25H42O2/c1-4-6-8-9-10-11-12-13-14-15-16-22(3)27-25(26)24-20-18-23(19-2
InchiKey:	YXXXDZMLZBSGFQ-UHFFFAOYSA-N
Formula:	C25H42O2
SMILES:	CCCCCCCCCCCC(C)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	374.60

Physical Properties

Property code	Value	Unit	Source
gf	26.04	kJ/mol	Joback Method
hf	-584.35	kJ/mol	Joback Method
hfus	53.42	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	7.886		Crippen Method
mvol	346.790	ml/mol	McGowan Method
pc	947.91	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	878.91	K	Joback Method
tc	1078.47	K	Joback Method
tf	467.61	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.24	J/molxK	878.91	Joback Method
cpg	1149.81	J/molxK	912.17	Joback Method
cpg	1168.12	J/molxK	945.43	Joback Method
cpg	1185.24	J/molxK	978.69	Joback Method
cpg	1201.20	J/molxK	1011.95	Joback Method
cpg	1216.06	J/molxK	1045.21	Joback Method
cpg	1229.87	J/molxK	1078.47	Joback Method
dvisc	0.0007290	Paxs	467.61	Joback Method

dvisc	0.0003164	Paxs	536.16	Joback Method
dvisc	0.0001659	Paxs	604.71	Joback Method
dvisc	0.0000992	Paxs	673.26	Joback Method
dvisc	0.0000653	Paxs	741.81	Joback Method
dvisc	0.0000461	Paxs	810.36	Joback Method
dvisc	0.0000344	Paxs	878.91	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=U299940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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