

4-Butyloxy-3-methylbenzoic acid, butyl ester

Other names:	Butyl 4-butoxy-3-methylbenzoate
Inchi:	InChI=1S/C16H24O3/c1-4-6-10-18-15-9-8-14(12-13(15)3)16(17)19-11-7-5-2/h8-9,12H,4-
InchiKey:	NSHTUZAELSBODY-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	CCCCOC(=O)c1ccc(OCCCC)c(C)c1
Mol. weight [g/mol]:	264.36

Physical Properties

Property code	Value	Unit	Source
gf	-161.93	kJ/mol	Joback Method
hf	-537.00	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.131		Crippen Method
mvol	225.850	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2032.00		NIST Webbook
tb	700.83	K	Joback Method
tc	896.69	K	Joback Method
tf	415.93	K	Joback Method
vc	0.866	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.88	J/molxK	700.83	Joback Method
cpg	644.40	J/molxK	733.47	Joback Method
cpg	660.01	J/molxK	766.12	Joback Method
cpg	674.73	J/molxK	798.76	Joback Method
cpg	688.57	J/molxK	831.40	Joback Method
cpg	701.53	J/molxK	864.05	Joback Method
cpg	713.61	J/molxK	896.69	Joback Method
dvisc	0.0008365	Paxs	415.93	Joback Method

dvisc	0.0004819	Paxs	463.41	Joback Method
dvisc	0.0003076	Paxs	510.90	Joback Method
dvisc	0.0002119	Paxs	558.38	Joback Method
dvisc	0.0001548	Paxs	605.86	Joback Method
dvisc	0.0001184	Paxs	653.35	Joback Method
dvisc	0.0000938	Paxs	700.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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