Amyl p-butoxybenzoate

Inchi: InChI=1S/C16H24O3/c1-3-5-7-13-19-16(17)14-8-10-15(11-9-14)18-12-6-4-2/h8-11H,3-7,
InchiKey: KGYDQHGMMFMZJP-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: CCCCCOC(=O)c1ccc(OCCCC)cc1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-152.30	kJ/mol	Joback Method
hf	-525.53	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.213		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2233.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	695.85	K	Joback Method
tc	890.88	K	Joback Method
tf	403.41	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.30	J/mol×K	695.85	Joback Method
cpg	702.45	J/mol×K	858.37	Joback Method
cpg	689.41	J/mol×K	825.87	Joback Method
cpg	675.49	J/mol×K	793.36	Joback Method
cpg	660.67	J/mol×K	760.86	Joback Method
cpg	644.95	J/mol×K	728.35	Joback Method

cpg	714.61	J/mol×K	890.88	Joback Method
dvisc	0.0000941	Pa×s	695.85	Joback Method
dvisc	0.0001205	Pa×s	647.11	Joback Method
dvisc	0.0001608	Pa×s	598.37	Joback Method
dvisc	0.0002257	Pa×s	549.63	Joback Method
dvisc	0.0003386	Pa×s	500.89	Joback Method
dvisc	0.0005542	Pa×s	452.15	Joback Method
dvisc	0.0010218	Pa×s	403.41	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R578782&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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