Heptyl p-butoxybenzoate

Inchi: InChI=1S/C18H28O3/c1-3-5-7-8-9-15-21-18(19)16-10-12-17(13-11-16)20-14-6-4-2/h10-1
InchiKey: ZJFJSQWZGMNYMD-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCCCCOC(=O)c1ccc(OCCCC)cc1
Mol. weight [g/mol]: 292.41

Physical Properties

Property code	Value	Unit	Source
gf	-135.46	kJ/mol	Joback Method
hf	-566.81	kJ/mol	Joback Method
hfus	40.00	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.993		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	2439.00		NIST Webbook
rinpol	2455.00		NIST Webbook
tb	741.61	K	Joback Method
tc	934.08	K	Joback Method
tf	425.95	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.43	J/mol×K	741.61	Joback Method
cpg	817.09	J/mol×K	902.00	Joback Method
cpg	803.67	J/mol×K	869.93	Joback Method
cpg	789.31	J/mol×K	837.85	Joback Method
cpg	774.00	J/mol×K	805.77	Joback Method

cpg	757.71	J/mol×K	773.69	Joback Method
cpg	829.58	J/mol×K	934.08	Joback Method
dvisc	0.0000735	Pa×s	741.61	Joback Method
dvisc	0.0000949	Pa×s	689.00	Joback Method
dvisc	0.0001278	Pa×s	636.39	Joback Method
dvisc	0.0001815	Pa×s	583.78	Joback Method
dvisc	0.0002763	Pa×s	531.17	Joback Method
dvisc	0.0004615	Pa×s	478.56	Joback Method
dvisc	0.0008747	Pa×s	425.95	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R578846&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