Benzoic acid, 3-(2-methoxyethyl)heptyl ester

Inchi: InChI=1S/C17H26O3/c1-3-4-8-15(11-13-19-2)12-14-20-17(18)16-9-6-5-7-10-16/h5-7,9-1
InchiKey: DQZUKUSMWHVXAM-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: CCCCC(CCOC)CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-136.69	kJ/mol	Joback Method
hf	-539.98	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.076		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2041.00		NIST Webbook
tb	713.31	K	Joback Method
tc	908.82	K	Joback Method
tf	387.16	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.64	J/mol×K	713.31	Joback Method
cpg	761.62	J/mol×K	876.24	Joback Method
cpg	748.17	J/mol×K	843.65	Joback Method
cpg	733.76	J/mol×K	811.07	Joback Method
cpg	718.39	J/mol×K	778.48	Joback Method
cpg	702.02	J/mol×K	745.90	Joback Method
cpg	774.14	J/mol×K	908.82	Joback Method
dvisc	0.0000771	Pa×s	713.31	Joback Method
dvisc	0.0001026	Pa×s	658.95	Joback Method

dvisc	0.0001438	Pa×s	604.59	Joback Method
dvisc	0.0002154	Pa×s	550.24	Joback Method
dvisc	0.0003526	Pa×s	495.88	Joback Method
dvisc	0.0006514	Pa×s	441.52	Joback Method
dvisc	0.0014301	Pa×s	387.16	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368698&Units=SI

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