m-Methoxybenzoic acid, octadecyl ester

Inchi: InChI=1S/C26H44O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-29-26(27)24-20-1
InchiKey: UBVGQHYZUPQEPU-UHFFFAOYSA-N
Formula: C26H44O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 404.63
CAS: 56954-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-68.10	kJ/mol	Joback Method
hf	-731.93	kJ/mol	Joback Method
hfus	60.72	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.114		Crippen Method
mcvol	366.750	ml/mol	McGowan Method
pc	881.04	kPa	Joback Method
rinpol	2974.50		NIST Webbook
tb	924.65	K	Joback Method
tc	1132.03	K	Joback Method
tf	516.11	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.64	J/mol×K	924.65	Joback Method
cpg	1307.96	J/mol×K	1097.47	Joback Method
cpg	1293.96	J/mol×K	1062.90	Joback Method
cpg	1278.67	J/mol×K	1028.34	Joback Method
cpg	1262.05	J/mol×K	993.78	Joback Method
cpg	1244.06	J/mol×K	959.21	Joback Method
cpg	1320.71	J/mol×K	1132.03	Joback Method
dvisc	0.0000241	Pa×s	924.65	Joback Method

dvisc	0.0000319	Pa×s	856.56	Joback Method
dvisc	0.0000441	Pa×s	788.47	Joback Method
dvisc	0.0000650	Pa×s	720.38	Joback Method
dvisc	0.0001039	Pa×s	652.29	Joback Method
dvisc	0.0001850	Pa×s	584.20	Joback Method
dvisc	0.0003838	Pa×s	516.11	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=C56954768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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