

o-Methoxybenzoic acid, decyl ester

Inchi:	InChI=1S/C18H28O3/c1-3-4-5-6-7-8-9-12-15-21-18(19)16-13-10-11-14-17(16)20-2/h10-1
InchiKey:	XFBRZOSYOJYTL-UHFFFAOYSA-N
Formula:	C18H28O3
SMILES:	CCCCCCCCCOC(=O)c1ccccc1OC
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
mvol	254.030	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2222.40		NIST Webbook
rinpol	2222.40		NIST Webbook
tb	741.61	K	Joback Method
tc	934.08	K	Joback Method
tf	425.95	K	Joback Method
vc	0.978	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.43	J/molxK	741.61	Joback Method
cpg	757.71	J/molxK	773.69	Joback Method
cpg	774.00	J/molxK	805.77	Joback Method
cpg	789.31	J/molxK	837.85	Joback Method
cpg	803.67	J/molxK	869.93	Joback Method
cpg	817.09	J/molxK	902.00	Joback Method
cpg	829.58	J/molxK	934.08	Joback Method
dvisc	0.0008747	Paxs	425.95	Joback Method

dvisc	0.0004615	Paxs	478.56	Joback Method
dvisc	0.0002763	Paxs	531.17	Joback Method
dvisc	0.0001815	Paxs	583.78	Joback Method
dvisc	0.0001278	Paxs	636.39	Joback Method
dvisc	0.0000949	Paxs	689.00	Joback Method
dvisc	0.0000735	Paxs	741.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U292301&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

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