

m-Anisic acid, 2-naphthyl ester

Inchi: InChI=1S/C18H14O3/c1-20-16-8-4-7-15(12-16)18(19)21-17-10-9-13-5-2-3-6-14(13)11-17
InchiKey: ZEKYQOAPVYHFEA-UHFFFAOYSA-N
Formula: C18H14O3
SMILES: COc1cccc(C(=O)Oc2ccc3ccccc3c2)c1
Mol. weight [g/mol]: 278.30

Physical Properties

Property code	Value	Unit	Source
gf	73.97	kJ/mol	Joback Method
hf	-150.68	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.068		Crippen Method
mcvol	210.810	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	2501.00		NIST Webbook
rinpol	2501.00		NIST Webbook
tb	792.25	K	Joback Method
tc	1040.33	K	Joback Method
tf	497.59	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.92	J/molxK	792.25	Joback Method
cpg	595.04	J/molxK	833.60	Joback Method
cpg	607.93	J/molxK	874.94	Joback Method
cpg	619.64	J/molxK	916.29	Joback Method
cpg	630.26	J/molxK	957.64	Joback Method
cpg	639.85	J/molxK	998.99	Joback Method
cpg	648.48	J/molxK	1040.33	Joback Method
dvisc	0.0007242	Paxs	497.59	Joback Method

dvisc	0.0004901	Paxs	546.70	Joback Method
dvisc	0.0003538	Paxs	595.81	Joback Method
dvisc	0.0002683	Paxs	644.92	Joback Method
dvisc	0.0002117	Paxs	694.03	Joback Method
dvisc	0.0001723	Paxs	743.14	Joback Method
dvisc	0.0001438	Paxs	792.25	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=U307805&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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