

m-Anisic acid, heptadecyl ester

Inchi:	InChI=1S/C25H42O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-28-25(26)23-19-18-2
InchiKey:	VYOKNZQHLOHEII-UHFFFAOYSA-N
Formula:	C25H42O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	390.60

Physical Properties

Property code	Value	Unit	Source
gf	-76.52	kJ/mol	Joback Method
hf	-711.29	kJ/mol	Joback Method
hfus	58.13	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.723		Crippen Method
mcvol	352.660	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinsol	2861.30		NIST Webbook
tb	901.77	K	Joback Method
tc	1104.50	K	Joback Method
tf	504.84	K	Joback Method
vc	1.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.73	J/molxK	901.77	Joback Method
cpg	1180.82	J/molxK	935.56	Joback Method
cpg	1198.58	J/molxK	969.35	Joback Method
cpg	1215.03	J/molxK	1003.14	Joback Method
cpg	1230.22	J/molxK	1036.92	Joback Method
cpg	1244.18	J/molxK	1070.71	Joback Method
cpg	1256.96	J/molxK	1104.50	Joback Method
dvisc	0.0004314	Paxs	504.84	Joback Method
dvisc	0.0002100	Paxs	571.00	Joback Method

dvisc	0.0001187	Paxs	637.15	Joback Method
dvisc	0.0000747	Paxs	703.30	Joback Method
dvisc	0.0000509	Paxs	769.46	Joback Method
dvisc	0.0000369	Paxs	835.61	Joback Method
dvisc	0.0000280	Paxs	901.77	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=U292258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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