1-(3,4-Dimethoxyphenyl)decane-3,5-diyl diacetate

Inchi: InChI=1S/C22H34O6/c1-6-7-8-9-19(27-16(2)23)15-20(28-17(3)24)12-10-18-11-13-21(25

InchiKey: QCJKXQWAFFZFLJ-UHFFFAOYSA-N

Formula: C22H34O6

SMILES: CCCCCC(CC(CCc1ccc(OC)c(OC)c1)OC(C)=O)OC(C)=O

Mol. weight [g/mol]: 394.50

CAS: 53254-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-455.21	kJ/mol	Joback Method
hf	-1048.42	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	90.52	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.470		Crippen Method
mcvol	323.700	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	2554.10		NIST Webbook
rinpol	2554.10		NIST Webbook
tb	935.94	K	Joback Method
tc	1147.69	K	Joback Method
tf	547.94	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.37	J/mol×K	935.94	Joback Method
cpg	1071.59	J/mol×K	971.23	Joback Method
cpg	1085.24	J/mol×K	1006.52	Joback Method
cpg	1097.32	J/mol×K	1041.82	Joback Method
cpg	1107.83	J/mol×K	1077.11	Joback Method
cpg	1116.75	J/mol×K	1112.40	Joback Method
cpg	1124.10	J/mol×K	1147.69	Joback Method

dvisc	0.0002477	Pa×s	547.94	Joback Method
dvisc	0.0001294	Pa×s	612.61	Joback Method
dvisc	0.0000765	Pa×s	677.27	Joback Method
dvisc	0.0000496	Pa×s	741.94	Joback Method
dvisc	0.0000345	Pa×s	806.61	Joback Method
dvisc	0.0000253	Pa×s	871.27	Joback Method
dvisc	0.0000194	Pa×s	935.94	Joback Method

Sources

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=C53254527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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