Sebacic acid, isohexyl 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C28H46O5/c1-24(2)14-13-21-32-27(29)17-11-6-4-5-7-12-18-28(30)33-23-20-2

InchiKey: ITSAITLOKYTRLJ-UHFFFAOYSA-N

Formula: C28H46O5

SMILES: COCCC(CCOC(=O)CCCCCCCCC(=O)OCCCC(C)C)c1ccccc1

Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-280.43	kJ/mol	Joback Method
hf	-1017.10	kJ/mol	Joback Method
hfus	62.03	kJ/mol	Joback Method
hvap	100.14	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.840		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	823.84	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1040.84	K	Joback Method
tc	1279.51	K	Joback Method
tf	568.29	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.68	J/mol×K	1040.84	Joback Method
cpg	1416.78	J/mol×K	1080.62	Joback Method
cpg	1431.88	J/mol×K	1120.40	Joback Method
cpg	1445.03	J/mol×K	1160.18	Joback Method
cpg	1456.29	J/mol×K	1199.96	Joback Method
cpg	1465.73	J/mol×K	1239.73	Joback Method
cpg	1473.40	J/mol×K	1279.51	Joback Method
dvisc	0.0002247	Pa×s	568.29	Joback Method

dvisc	0.0000972	Pa×s	647.05	Joback Method
dvisc	0.0000504	Pa×s	725.81	Joback Method
dvisc	0.0000297	Pa×s	804.57	Joback Method
dvisc	0.0000193	Pa×s	883.32	Joback Method
dvisc	0.0000134	Pa×s	962.08	Joback Method
dvisc	0.0000099	Pa×s	1040.84	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=U355483&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