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

Inchi: InChI=1S/C29H48O5/c1-3-4-5-10-16-23-33-28(30)19-14-8-6-7-9-15-20-29(31)34-25-22-2

InchiKey: PVUQETBHMVLULK-UHFFFAOYSA-N

Formula: C29H48O5

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCCC(CCOC)c1ccccc1

Mol. weight [g/mol]: 476.69

Physical Properties

Property code	Value	Unit	Source
gf	-269.57	kJ/mol	Joback Method
hf	-1032.46	kJ/mol	Joback Method
hfus	68.15	kJ/mol	Joback Method
hvap	102.76	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.374		Crippen Method
mcvol	416.460	ml/mol	McGowan Method
pc	776.77	kPa	Joback Method
rinpol	3387.00		NIST Webbook
rinpol	3387.00		NIST Webbook
tb	1064.16	K	Joback Method
tc	1314.18	K	Joback Method
tf	594.56	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.49	J/mol×K	1064.16	Joback Method
cpg	1480.02	J/mol×K	1105.83	Joback Method
cpg	1495.35	J/mol×K	1147.50	Joback Method
cpg	1508.57	J/mol×K	1189.17	Joback Method
cpg	1519.74	J/mol×K	1230.84	Joback Method
cpg	1528.95	J/mol×K	1272.51	Joback Method
cpg	1536.27	J/mol×K	1314.18	Joback Method
dvisc	0.0001760	Pa×s	594.56	Joback Method

dvisc	0.0000809	Pa×s	672.83	Joback Method
dvisc	0.0000437	Pa×s	751.09	Joback Method
dvisc	0.0000266	Pa×s	829.36	Joback Method
dvisc	0.0000176	Pa×s	907.63	Joback Method
dvisc	0.0000124	Pa×s	985.89	Joback Method
dvisc	0.0000092	Pa×s	1064.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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