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

Inchi: InChI=1S/C26H42O5/c1-3-4-20-30-25(27)16-12-7-5-6-8-13-17-26(28)31-22-19-24(18-21

InchiKey: NQXINURPQALJAZ-UHFFFAOYSA-N

Formula: C26H42O5

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

Mol. weight [g/mol]: 434.61

Physical Properties

Property code	Value	Unit	Source
gf	-294.83	kJ/mol	Joback Method
hf	-970.54	kJ/mol	Joback Method
hfus	60.38	kJ/mol	Joback Method
hvap	96.08	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.204		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
rinpol	3089.00		NIST Webbook
tb	995.52	K	Joback Method
tc	1219.91	K	Joback Method
tf	560.75	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.13	J/mol×K	995.52	Joback Method
cpg	1290.98	J/mol×K	1032.92	Joback Method
cpg	1306.09	J/mol×K	1070.32	Joback Method
cpg	1319.51	J/mol×K	1107.71	Joback Method
cpg	1331.30	J/mol×K	1145.11	Joback Method
cpg	1341.49	J/mol×K	1182.51	Joback Method
cpg	1350.12	J/mol×K	1219.91	Joback Method
dvisc	0.0002634	Pa×s	560.75	Joback Method
dvisc	0.0001241	Pa×s	633.21	Joback Method

dvisc	0.0000682	Pa×s	705.67	Joback Method
dvisc	0.0000419	Pa×s	778.13	Joback Method
dvisc	0.0000280	Pa×s	850.60	Joback Method
dvisc	0.0000199	Pa×s	923.06	Joback Method
dvisc	0.0000149	Pa×s	995.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355482&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