Sebacic acid, heptyl 4-methoxy-2-methylbutyl ester

Other names: Sebacic acid, heptyl 4-methoxy-2-methylphenyl ester
Inchi: InChI=1S/C23H44O5/c1-4-5-6-11-14-18-27-22(24)15-12-9-7-8-10-13-16-23(25)28-20-21
InchiKey: WVEFKGOFWFZHAJ-UHFFFAOYSA-N
Formula: C23H44O5
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]: 400.59

Physical Properties

Property code	Value	Unit	Source
gf	-432.50	kJ/mol	Joback Method
hf	-1145.15	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.837		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	2753.00		NIST Webbook
tb	900.20	K	Joback Method
tc	1102.87	K	Joback Method
tf	500.52	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.09	J/mol×K	900.20	Joback Method
cpg	1269.34	J/mol×K	1069.09	Joback Method
cpg	1255.73	J/mol×K	1035.31	Joback Method
cpg	1240.71	J/mol×K	1001.53	Joback Method
cpg	1224.28	J/mol×K	967.76	Joback Method
cpg	1206.41	J/mol×K	933.98	Joback Method
cpg	1281.58	J/mol×K	1102.87	Joback Method
dvisc	0.0000231	Pa×s	900.20	Joback Method

dvisc	0.0000312	Pa×s	833.59	Joback Method
dvisc	0.0000444	Pa×s	766.97	Joback Method
dvisc	0.0000674	Pa×s	700.36	Joback Method
dvisc	0.0001118	Pa×s	633.75	Joback Method
dvisc	0.0002090	Pa×s	567.13	Joback Method
dvisc	0.0004611	Pa×s	500.52	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=U355327&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