Sebacic acid, 4-methylhept-3-yl pentyl ester

Inchi: InChI=1S/C23H44O4/c1-5-8-15-19-26-22(24)17-13-11-9-10-12-14-18-23(25)27-21(7-3)2
InchiKey: PKLJKBRKYRFJCT-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-329.94	kJ/mol	Joback Method
hf	-1018.21	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.599		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	877.34	K	Joback Method
tc	1074.11	K	Joback Method
tf	463.29	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.40	J/mol×K	877.34	Joback Method
cpg	1174.99	J/mol×K	910.14	Joback Method
cpg	1193.27	J/mol×K	942.93	Joback Method
cpg	1210.26	J/mol×K	975.73	Joback Method
cpg	1226.01	J/mol×K	1008.52	Joback Method
cpg	1240.52	J/mol×K	1041.32	Joback Method
cpg	1253.84	J/mol×K	1074.11	Joback Method
dvisc	0.0008160	Pa×s	463.29	Joback Method

dvisc	0.0003252	Pa×s	532.30	Joback Method
dvisc	0.0001600	Pa×s	601.31	Joback Method
dvisc	0.0000911	Pa×s	670.32	Joback Method
dvisc	0.0000577	Pa×s	739.32	Joback Method
dvisc	0.0000394	Pa×s	808.33	Joback Method
dvisc	0.0000286	Pa×s	877.34	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=U416199&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

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