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

Inchi: InChI=1S/C25H48O4/c1-5-8-9-14-17-21-28-24(26)19-15-12-10-11-13-16-20-25(27)29-23
InchiKey: LMONUZWICIQRJV-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-313.10	kJ/mol	Joback Method
hf	-1059.49	kJ/mol	Joback Method
hfus	59.03	kJ/mol	Joback Method
hvap	88.78	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.379		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	923.10	K	Joback Method
tc	1132.09	K	Joback Method
tf	485.83	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.95	J/mol×K	923.10	Joback Method
cpg	1302.47	J/mol×K	957.93	Joback Method
cpg	1321.46	J/mol×K	992.76	Joback Method
cpg	1338.96	J/mol×K	1027.60	Joback Method
cpg	1355.01	J/mol×K	1062.43	Joback Method
cpg	1369.65	J/mol×K	1097.26	Joback Method
cpg	1382.92	J/mol×K	1132.09	Joback Method
dvisc	0.0006234	Pa×s	485.83	Joback Method

dvisc	0.0002451	Pa×s	558.71	Joback Method
dvisc	0.0001196	Pa×s	631.59	Joback Method
dvisc	0.0000676	Pa×s	704.47	Joback Method
dvisc	0.0000426	Pa×s	777.34	Joback Method
dvisc	0.0000290	Pa×s	850.22	Joback Method
dvisc	0.0000210	Pa×s	923.10	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=U416201&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