Sebacic acid, di(2,4-dimethylpent-3-yl) ester

Inchi: InChI=1S/C24H46O4/c1-17(2)23(18(3)4)27-21(25)15-13-11-9-10-12-14-16-22(26)28-24(
InchiKey: QETADEVOTHFWPS-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CC(C)C(OC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-331.28	kJ/mol	Joback Method
hf	-1059.97	kJ/mol	Joback Method
hfus	42.35	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.555		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	874.28	kPa	Joback Method
rinpol	2490.00		NIST Webbook
rinpol	2490.00		NIST Webbook
tb	898.46	K	Joback Method
tc	1100.12	K	Joback Method
tf	414.56	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.09	J/mol×K	898.46	Joback Method
cpg	1239.98	J/mol×K	932.07	Joback Method
cpg	1258.41	J/mol×K	965.68	Joback Method
cpg	1275.43	J/mol×K	999.29	Joback Method
cpg	1291.07	J/mol×K	1032.90	Joback Method
cpg	1305.37	J/mol×K	1066.51	Joback Method
cpg	1318.35	J/mol×K	1100.12	Joback Method
dvisc	0.0016886	Pa×s	414.56	Joback Method

dvisc	0.0004213	Pa×s	495.21	Joback Method
dvisc	0.0001551	Pa×s	575.86	Joback Method
dvisc	0.0000730	Pa×s	656.51	Joback Method
dvisc	0.0000405	Pa×s	737.16	Joback Method
dvisc	0.0000252	Pa×s	817.81	Joback Method
dvisc	0.0000171	Pa×s	898.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355441&Units=SI

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