Sebacic acid, 2,4-dimethylpent-3-yl heptyl ester

Inchi: InChI=1S/C24H46O4/c1-6-7-8-13-16-19-27-22(25)17-14-11-9-10-12-15-18-23(26)28-24(

InchiKey: WEHGGWBCMGXWCU-UHFFFAOYSA-N

Formula: C24H46O4

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-323.96	kJ/mol	Joback Method
hf	-1044.13	kJ/mol	Joback Method
hfus	52.92	kJ/mol	Joback Method
hvap	86.17	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.845		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2625.00		NIST Webbook
tb	899.78	K	Joback Method
tc	1101.76	K	Joback Method
tf	459.56	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.83	J/mol×K	899.78	Joback Method
cpg	1238.81	J/mol×K	933.44	Joback Method
cpg	1257.37	J/mol×K	967.11	Joback Method
cpg	1274.54	J/mol×K	1000.77	Joback Method
cpg	1290.36	J/mol×K	1034.43	Joback Method
cpg	1304.87	J/mol×K	1068.10	Joback Method
cpg	1318.09	J/mol×K	1101.76	Joback Method
dvisc	0.0008558	Pa×s	459.56	Joback Method
dvisc	0.0003072	Pa×s	532.93	Joback Method

dvisc	0.0001413	Pa×s	606.30	Joback Method
dvisc	0.0000768	Pa×s	679.67	Joback Method
dvisc	0.0000471	Pa×s	753.04	Joback Method
dvisc	0.0000314	Pa×s	826.41	Joback Method
dvisc	0.0000224	Pa×s	899.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355430&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