Sebacic acid, 3,3-dimethylbut-2-yl pentyl ester

Inchi: InChI=1S/C21H40O4/c1-6-7-14-17-24-19(22)15-12-10-8-9-11-13-16-20(23)25-18(2)21(3
InchiKey: DNKKTVLGGKHXEB-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.50	kJ/mol	Joback Method
hf	-980.40	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.818		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	828.79	K	Joback Method
tc	1018.11	K	Joback Method
tf	458.17	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.48	J/mol×K	828.79	Joback Method
cpg	1050.15	J/mol×K	860.34	Joback Method
cpg	1067.69	J/mol×K	891.90	Joback Method
cpg	1084.15	J/mol×K	923.45	Joback Method
cpg	1099.56	J/mol×K	955.00	Joback Method
cpg	1113.95	J/mol×K	986.55	Joback Method
cpg	1127.36	J/mol×K	1018.11	Joback Method
dvisc	0.0008434	Pa×s	458.17	Joback Method

dvisc	0.0003582	Pa×s	519.94	Joback Method
dvisc	0.0001825	Pa×s	581.71	Joback Method
dvisc	0.0001058	Pa×s	643.48	Joback Method
dvisc	0.0000675	Pa×s	705.25	Joback Method
dvisc	0.0000463	Pa×s	767.02	Joback Method
dvisc	0.0000336	Pa×s	828.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355598&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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