Sebacic acid, decyl neopentyl ester

Inchi: InChI=1S/C25H48O4/c1-5-6-7-8-9-12-15-18-21-28-23(26)19-16-13-10-11-14-17-20-24(2
InchiKey: QXFFZSZGIXCOCM-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-305.38	kJ/mol	Joback Method
hf	-1057.68	kJ/mol	Joback Method
hfus	58.67	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.380		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	2823.00		NIST Webbook
tb	920.75	K	Joback Method
tc	1128.53	K	Joback Method
tf	518.25	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.05	J/mol×K	920.75	Joback Method
cpg	1369.40	J/mol×K	1093.90	Joback Method
cpg	1354.32	J/mol×K	1059.27	Joback Method
cpg	1338.00	J/mol×K	1024.64	Joback Method
cpg	1320.39	J/mol×K	990.01	Joback Method
cpg	1301.43	J/mol×K	955.38	Joback Method
cpg	1383.30	J/mol×K	1128.53	Joback Method
dvisc	0.0000195	Pa×s	920.75	Joback Method
dvisc	0.0000265	Pa×s	853.67	Joback Method

dvisc	0.0000382	Pa×s	786.58	Joback Method
dvisc	0.0000588	Pa×s	719.50	Joback Method
dvisc	0.0000990	Pa×s	652.42	Joback Method
dvisc	0.0001876	Pa×s	585.33	Joback Method
dvisc	0.0004198	Pa×s	518.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U354471&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