Sebacic acid, di(4-methylhept-3-yl) ester

Inchi: InChI=1S/C26H50O4/c1-7-17-21(5)23(9-3)29-25(27)19-15-13-11-12-14-16-20-26(28)30-
InchiKey: MXDDGCDWTPVWPJ-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCC(C)C(CC)OC(=O)CCCCCCCCC(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-309.56	kJ/mol	Joback Method
hf	-1090.69	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.623		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	775.91	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	945.10	K	Joback Method
tc	1159.56	K	Joback Method
tf	467.10	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.69	J/mol×K	945.10	Joback Method
cpg	1367.44	J/mol×K	980.84	Joback Method
cpg	1386.54	J/mol×K	1016.59	Joback Method
cpg	1404.03	J/mol×K	1052.33	Joback Method
cpg	1419.96	J/mol×K	1088.07	Joback Method
cpg	1434.37	J/mol×K	1123.82	Joback Method
cpg	1447.31	J/mol×K	1159.56	Joback Method
dvisc	0.0007744	Pa×s	467.10	Joback Method

dvisc	0.0002483	Pa×s	546.77	Joback Method
dvisc	0.0001063	Pa×s	626.43	Joback Method
dvisc	0.0000551	Pa×s	706.10	Joback Method
dvisc	0.0000327	Pa×s	785.77	Joback Method
dvisc	0.0000213	Pa×s	865.43	Joback Method
dvisc	0.0000149	Pa×s	945.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416207&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