

Sebacic acid, di(6-methylhept-2-yl) ester

Inchi: InChI=1S/C26H50O4/c1-21(2)15-13-17-23(5)29-25(27)19-11-9-7-8-10-12-20-26(28)30-2
InchiKey: BKEWEIYKDTTWRH-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CC(C)CCCC(C)OC(=O)CCCCCCCC(=O)OC(C)CCCC(C)C
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	2653.00		NIST Webbook
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tb	945.10	K	Joback Method
tc	1159.56	K	Joback Method
tf	467.10	K	Joback Method
vc	1.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.69	J/molxK	945.10	Joback Method
cpg	1434.37	J/molxK	1123.82	Joback Method
cpg	1419.96	J/molxK	1088.07	Joback Method
cpg	1404.03	J/molxK	1052.33	Joback Method
cpg	1386.54	J/molxK	1016.59	Joback Method
cpg	1367.44	J/molxK	980.84	Joback Method
cpg	1447.31	J/molxK	1159.56	Joback Method
dvisc	0.0000149	Paxs	945.10	Joback Method

dvisc	0.0000213	Paxs	865.43	Joback Method
dvisc	0.0000327	Paxs	785.77	Joback Method
dvisc	0.0000551	Paxs	706.10	Joback Method
dvisc	0.0001063	Paxs	626.43	Joback Method
dvisc	0.0002483	Paxs	546.77	Joback Method
dvisc	0.0007744	Paxs	467.10	Joback Method

Sources

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=U416225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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