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

Inchi: InChI=1S/C21H40O4/c1-16(2)15-24-19(22)13-11-9-7-8-10-12-14-20(23)25-21(17(3)4)18

InchiKey: IGBMTVOWDIDJSZ-UHFFFAOYSA-N

Formula: C21H40O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-351.66	kJ/mol	Joback Method
hf	-987.49	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.530		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	830.70	K	Joback Method
tc	1020.47	K	Joback Method
tf	410.75	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.14	J/mol×K	830.70	Joback Method
cpg	1051.06	J/mol×K	862.33	Joback Method
cpg	1068.79	J/mol×K	893.96	Joback Method
cpg	1085.37	J/mol×K	925.58	Joback Method
cpg	1100.82	J/mol×K	957.21	Joback Method
cpg	1115.14	J/mol×K	988.84	Joback Method
cpg	1128.36	J/mol×K	1020.47	Joback Method
dvisc	0.0016234	Pa×s	410.75	Joback Method

dvisc	0.0005267	Pa×s	480.74	Joback Method
dvisc	0.0002275	Pa×s	550.73	Joback Method
dvisc	0.0001187	Pa×s	620.73	Joback Method
dvisc	0.0000707	Pa×s	690.72	Joback Method
dvisc	0.0000463	Pa×s	760.71	Joback Method
dvisc	0.0000326	Pa×s	830.70	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=U355425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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