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

Inchi: InChI=1S/C19H34O5/c1-4-5-12-15-23-18(21)13-10-8-6-7-9-11-14-19(22)24-17(3)16(2)20

InchiKey: DPPUDCSLCKUWAE-UHFFFAOYSA-N

Formula: C19H34O5

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O

Mol. weight [g/mol]: 342.47

Physical Properties

Property code	Value	Unit	Source
gf	-490.10	kJ/mol	Joback Method
hf	-1042.95	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.361		Crippen Method
mcvol	295.020	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	2363.00		NIST Webbook
tb	840.13	K	Joback Method
tc	1031.64	K	Joback Method
tf	483.14	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.24	J/mol×K	840.13	Joback Method
cpg	1004.05	J/mol×K	999.72	Joback Method
cpg	991.79	J/mol×K	967.80	Joback Method
cpg	978.50	J/mol×K	935.88	Joback Method
cpg	964.15	J/mol×K	903.97	Joback Method
cpg	948.74	J/mol×K	872.05	Joback Method
cpg	1015.28	J/mol×K	1031.64	Joback Method
dvisc	0.0000537	Pa×s	840.13	Joback Method
dvisc	0.0000713	Pa×s	780.63	Joback Method

dvisc	0.0000991	Pa×s	721.13	Joback Method
dvisc	0.0001463	Pa×s	661.63	Joback Method
dvisc	0.0002331	Pa×s	602.14	Joback Method
dvisc	0.0004114	Pa×s	542.64	Joback Method
dvisc	0.0008351	Pa×s	483.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355776&Units=SI

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