Glutaric acid, octyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C21H40O4/c1-6-7-8-9-10-11-15-24-19(22)13-12-14-20(23)25-17-18(2)16-21(3
InchiKey: SCMJEDLWCYNEOW-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.50	kJ/mol	Joback Method
hf	-980.40	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.676		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2362.00		NIST Webbook
tb	828.79	K	Joback Method
tc	1018.11	K	Joback Method
tf	458.17	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.48	J/mol×K	828.79	Joback Method
cpg	1050.15	J/mol×K	860.34	Joback Method
cpg	1067.69	J/mol×K	891.90	Joback Method
cpg	1084.15	J/mol×K	923.45	Joback Method
cpg	1099.56	J/mol×K	955.00	Joback Method
cpg	1113.95	J/mol×K	986.55	Joback Method
cpg	1127.36	J/mol×K	1018.11	Joback Method
dvisc	0.0008434	Pa×s	458.17	Joback Method
dvisc	0.0003582	Pa×s	519.94	Joback Method

dvisc	0.0001825	Pa×s	581.71	Joback Method
dvisc	0.0001058	Pa×s	643.48	Joback Method
dvisc	0.0000675	Pa×s	705.25	Joback Method
dvisc	0.0000463	Pa×s	767.02	Joback Method
dvisc	0.0000336	Pa×s	828.79	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=U377228&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