Glutaric acid, di((2-methylcyclohex-1-enyl)methyl) ester

Inchi: InChI=1S/C21H32O4/c1-16-8-3-5-10-18(16)14-24-20(22)12-7-13-21(23)25-15-19-11-6-4-9-17(19)2/h14-15H,3-13H2,1-2H3

InchiKey: WORXIMRANCBTAC-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: CC1=C(COC(=O)CCCC(=O)OCC2=C(C)CCCC2)CCCC1

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-256.18	kJ/mol	Joback Method
hf	-747.37	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.024		Crippen Method
mcvol	291.310	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook
tb	899.14	K	Joback Method
tc	1118.28	K	Joback Method
tf	545.59	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.50	J/mol×K	899.14	Joback Method
cpg	973.53	J/mol×K	935.66	Joback Method
cpg	989.04	J/mol×K	972.19	Joback Method
cpg	1003.05	J/mol×K	1008.71	Joback Method
cpg	1015.60	J/mol×K	1045.23	Joback Method
cpg	1026.71	J/mol×K	1081.76	Joback Method
cpg	1036.41	J/mol×K	1118.28	Joback Method
dvisc	0.0004059	Pa×s	545.59	Joback Method

dvisc	0.0002222	Pa×s	604.51	Joback Method
dvisc	0.0001354	Pa×s	663.44	Joback Method
dvisc	0.0000895	Pa×s	722.37	Joback Method
dvisc	0.0000629	Pa×s	781.29	Joback Method
dvisc	0.0000465	Pa×s	840.21	Joback Method
dvisc	0.0000357	Pa×s	899.14	Joback Method

Sources

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=U405512&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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