Glutaric acid, 2,4-dimethylpent-3-yl tetradecyl ester

Inchi: InChI=1S/C26H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-21-29-24(27)19-18-20-25(28)
InchiKey: VPECGRUDCZDFMW-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-307.12	kJ/mol	Joback Method
hf	-1085.41	kJ/mol	Joback Method
hfus	58.10	kJ/mol	Joback Method
hvap	90.62	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.625		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	945.54	K	Joback Method
tc	1161.05	K	Joback Method
tf	482.10	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.32	J/mol×K	945.54	Joback Method
cpg	1367.21	J/mol×K	981.46	Joback Method
cpg	1386.45	J/mol×K	1017.38	Joback Method
cpg	1404.07	J/mol×K	1053.29	Joback Method
cpg	1420.12	J/mol×K	1089.21	Joback Method
cpg	1434.66	J/mol×K	1125.13	Joback Method
cpg	1447.72	J/mol×K	1161.05	Joback Method
dvisc	0.0006421	Pa×s	482.10	Joback Method
dvisc	0.0002284	Pa×s	559.34	Joback Method

dvisc	0.0001044	Pa×s	636.58	Joback Method
dvisc	0.0000565	Pa×s	713.82	Joback Method
dvisc	0.0000345	Pa×s	791.06	Joback Method
dvisc	0.0000230	Pa×s	868.30	Joback Method
dvisc	0.0000164	Pa×s	945.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359486&Units=SI
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

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

Latest version available from:
https://www.chemeo.com/cid/24-728-7/Glutaric-acid-2-4-dimethylpent-3-yl-tetradecyl-ester.pdf
Generated by Cheméo on 2024-10-12 04:08:14.568977916 +0000 UTC m=+3286957.205947165.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.