

Glutaric acid, 4-heptyl tridecyl ester

Inchi: InChI=1S/C25H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-22-28-24(26)20-17-21-25(27)29-30
InchiKey: VHPKVXDFIIBTDL-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CCC)CCC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-310.66	kJ/mol	Joback Method
hf	-1054.21	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.523		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	923.54	K	Joback Method
tc	1133.47	K	Joback Method
tf	500.83	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.56	J/molxK	923.54	Joback Method
cpg	1302.20	J/molxK	958.53	Joback Method
cpg	1321.30	J/molxK	993.52	Joback Method
cpg	1338.92	J/molxK	1028.50	Joback Method
cpg	1355.09	J/molxK	1063.49	Joback Method
cpg	1369.84	J/molxK	1098.48	Joback Method
cpg	1383.23	J/molxK	1133.47	Joback Method
dvisc	0.0005334	Paxs	500.83	Joback Method

dvisc	0.0002287	Paxs	571.28	Joback Method
dvisc	0.0001181	Paxs	641.73	Joback Method
dvisc	0.0000695	Paxs	712.18	Joback Method
dvisc	0.0000450	Paxs	782.64	Joback Method
dvisc	0.0000313	Paxs	853.09	Joback Method
dvisc	0.0000230	Paxs	923.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	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.cheméo.com/cid/19-155-9/Glutaric-acid-4-heptyl-tridecyl-ester.pdf>

Generated by Cheméo on 2024-04-27 10:03:58.353598341 +0000 UTC m=+16501487.274175658.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.