

Glutaric acid, heptadecyl phenethyl ester

Inchi: InChI=1S/C30H50O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-26-33-29(31)23-20-24-30
InchiKey: NUKQMRACJWVUMJ-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-153.71	kJ/mol	Joback Method
hf	-915.60	kJ/mol	Joback Method
hfus	73.07	kJ/mol	Joback Method
hvap	102.96	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.357		Crippen Method
mvol	424.680	ml/mol	McGowan Method
pc	740.43	kPa	Joback Method
rinpol	3614.00		NIST Webbook
tb	1065.06	K	Joback Method
tc	1318.01	K	Joback Method
tf	598.60	K	Joback Method
vc	1.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.54	J/molxK	1065.06	Joback Method
cpg	1516.81	J/molxK	1107.22	Joback Method
cpg	1534.05	J/molxK	1149.38	Joback Method
cpg	1549.38	J/molxK	1191.53	Joback Method
cpg	1562.89	J/molxK	1233.69	Joback Method
cpg	1574.70	J/molxK	1275.85	Joback Method
cpg	1584.92	J/molxK	1318.01	Joback Method
dvisc	0.0002069	Paxs	598.60	Joback Method
dvisc	0.0000977	Paxs	676.34	Joback Method

dvisc	0.0000539	Paxs	754.09	Joback Method
dvisc	0.0000332	Paxs	831.83	Joback Method
dvisc	0.0000222	Paxs	909.57	Joback Method
dvisc	0.0000159	Paxs	987.32	Joback Method
dvisc	0.0000119	Paxs	1065.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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