

Glutaric acid, cyclohexylmethyl tetradecyl ester

Inchi:	InChI=1S/C26H48O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-22-29-25(27)20-17-21-26(28)30-23
InchiKey:	CSDUZVCIQOVARZ-UHFFFAOYSA-N
Formula:	C26H48O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	424.66

Physical Properties

Property code	Value	Unit	Source
gf	-275.35	kJ/mol	Joback Method
hf	-1015.25	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.524		Crippen Method
mcvol	381.220	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	966.41	K	Joback Method
tc	1184.04	K	Joback Method
tf	534.48	K	Joback Method
vc	1.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1342.26	J/molxK	966.41	Joback Method
cpg	1362.22	J/molxK	1002.68	Joback Method
cpg	1380.42	J/molxK	1038.95	Joback Method
cpg	1396.91	J/molxK	1075.23	Joback Method
cpg	1411.74	J/molxK	1111.50	Joback Method
cpg	1424.96	J/molxK	1147.77	Joback Method
cpg	1436.62	J/molxK	1184.04	Joback Method
dvisc	0.0004565	Paxs	534.48	Joback Method

dvisc	0.0002044	Paxs	606.47	Joback Method
dvisc	0.0001085	Paxs	678.46	Joback Method
dvisc	0.0000650	Paxs	750.44	Joback Method
dvisc	0.0000426	Paxs	822.43	Joback Method
dvisc	0.0000299	Paxs	894.42	Joback Method
dvisc	0.0000221	Paxs	966.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391638&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

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
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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