

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

Inchi: CC1=C(COC(=O)CCCC(=O)OC(C)C(C)C)CCCC1
InchiKey: CAKDCMSLMYFZON-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: CC1=C(COC(=O)CCCC(=O)OC(C)C(C)C)CCCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-329.18	kJ/mol	Joback Method
hf	-805.51	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.178		Crippen Method
mvol	264.200	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	796.28	K	Joback Method
tc	998.66	K	Joback Method
tf	444.36	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.39	J/molxK	796.28	Joback Method
cpg	834.05	J/molxK	830.01	Joback Method
cpg	850.50	J/molxK	863.74	Joback Method
cpg	865.78	J/molxK	897.47	Joback Method
cpg	879.89	J/molxK	931.20	Joback Method
cpg	892.85	J/molxK	964.93	Joback Method
cpg	904.67	J/molxK	998.66	Joback Method
dvisc	0.0010379	Paxs	444.36	Joback Method

dvisc	0.0004734	Paxs	503.01	Joback Method
dvisc	0.0002544	Paxs	561.67	Joback Method
dvisc	0.0001538	Paxs	620.32	Joback Method
dvisc	0.0001014	Paxs	678.97	Joback Method
dvisc	0.0000714	Paxs	737.63	Joback Method
dvisc	0.0000530	Paxs	796.28	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=U405502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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