Glutaric acid, (2-methylcyclohex-1-enyl)methyl hept-2-yl ester

Inchi: InChI=1S/C20H34O4/c1-4-5-6-11-17(3)24-20(22)14-9-13-19(21)23-15-18-12-8-7-10-16(1

InchiKey: CWMNUSXCTVHAGX-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC1=C(C)CCCC1

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-309.90	kJ/mol	Joback Method
hf	-841.51	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.102		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2297.00		NIST Webbook
tb	842.48	K	Joback Method
tc	1042.81	K	Joback Method
tf	481.90	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.80	J/mol×K	842.48	Joback Method
cpg	952.54	J/mol×K	875.87	Joback Method
cpg	969.04	J/mol×K	909.26	Joback Method
cpg	984.32	J/mol×K	942.64	Joback Method
cpg	998.39	J/mol×K	976.03	Joback Method
cpg	1011.27	J/mol×K	1009.42	Joback Method
cpg	1022.99	J/mol×K	1042.81	Joback Method
dvisc	0.0007030	Pa×s	481.90	Joback Method
dvisc	0.0003412	Pa×s	542.00	Joback Method

dvisc	0.0001913	Pa×s	602.09	Joback Method
dvisc	0.0001192	Pa×s	662.19	Joback Method
dvisc	0.0000803	Pa×s	722.29	Joback Method
dvisc	0.0000575	Pa×s	782.38	Joback Method
dvisc	0.0000432	Pa×s	842.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405504&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

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