Glutaric acid, heptyl pent-4-enyl ester

Inchi: InChI=1S/C17H30O4/c1-3-5-7-8-10-15-21-17(19)13-11-12-16(18)20-14-9-6-4-2/h4H,2-3,
InchiKey: ULEXLLOHSBEZCF-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: C=CCCCOC(=O)CCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-287.74	kJ/mol	Joback Method
hf	-758.38	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2096.00		NIST Webbook
tb	737.62	K	Joback Method
tc	916.09	K	Joback Method
tf	423.91	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.83	J/mol×K	737.62	Joback Method
cpg	782.30	J/mol×K	767.36	Joback Method
cpg	797.92	J/mol×K	797.11	Joback Method
cpg	812.71	J/mol×K	826.85	Joback Method
cpg	826.68	J/mol×K	856.60	Joback Method
cpg	839.84	J/mol×K	886.34	Joback Method
cpg	852.20	J/mol×K	916.09	Joback Method
dvisc	0.0011463	Pa×s	423.91	Joback Method
dvisc	0.0005872	Pa×s	476.20	Joback Method

dvisc	0.0003434	Pa×s	528.48	Joback Method
dvisc	0.0002212	Pa×s	580.77	Joback Method
dvisc	0.0001532	Pa×s	633.05	Joback Method
dvisc	0.0001122	Pa×s	685.34	Joback Method
dvisc	0.0000859	Pa×s	737.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359986&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