Adipic acid, heptyl trans-hex-3-enyl ester

Inchi: InChI=1S/C19H34O4/c1-3-5-7-9-13-17-23-19(21)15-11-10-14-18(20)22-16-12-8-6-4-2/h6
InchiKey: QLHHPAJQCMLCGM-SOFGYWHQSA-N
Formula: C19H34O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-278.52	kJ/mol	Joback Method
hf	-807.87	kJ/mol	Joback Method
hfus	50.74	kJ/mol	Joback Method
hvap	76.16	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2229.00		NIST Webbook
tb	790.86	K	Joback Method
tc	974.63	K	Joback Method
tf	443.13	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.09	J/mol×K	790.86	Joback Method
cpg	901.36	J/mol×K	821.49	Joback Method
cpg	917.69	J/mol×K	852.12	Joback Method
cpg	933.10	J/mol×K	882.74	Joback Method
cpg	947.61	J/mol×K	913.37	Joback Method
cpg	961.25	J/mol×K	944.00	Joback Method
cpg	974.04	J/mol×K	974.63	Joback Method
dvisc	0.0008689	Pa×s	443.13	Joback Method
dvisc	0.0004171	Pa×s	501.08	Joback Method

dvisc	0.0002331	Pa×s	559.04	Joback Method
dvisc	0.0001453	Pa×s	617.00	Joback Method
dvisc	0.0000983	Pa×s	674.95	Joback Method
dvisc	0.0000707	Pa×s	732.90	Joback Method
dvisc	0.0000533	Pa×s	790.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354011&Units=SI

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