Adipic acid, heptadecyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C28H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-31-27(29)21-18-19

InchiKey: RKOADGRXACZHPJ-UHFFFAOYSA-N

Formula: C28H52O4

SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-203.67	kJ/mol	Joback Method
hf	-995.21	kJ/mol	Joback Method
hfus	71.26	kJ/mol	Joback Method
hvap	95.64	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	704.71	kPa	Joback Method
rinpol	3130.00		NIST Webbook
tb	989.18	K	Joback Method
tc	1224.31	K	Joback Method
tf	533.92	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.87	J/mol×K	989.18	Joback Method
cpg	1465.85	J/mol×K	1028.37	Joback Method
cpg	1485.96	J/mol×K	1067.56	Joback Method
cpg	1504.28	J/mol×K	1106.74	Joback Method
cpg	1520.89	J/mol×K	1145.93	Joback Method
cpg	1535.88	J/mol×K	1185.12	Joback Method
cpg	1549.31	J/mol×K	1224.31	Joback Method

Sources

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=U354040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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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