Fumaric acid, 3-methylbut-3-enyl pentadecyl ester

Inchi: InChI=1S/C24H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-27-23(25)17-18-24(26)28
InchiKey: MIXKGVXNMGZURA-ISLYRVAYSA-N
Formula: C24H42O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-157.13	kJ/mol	Joback Method
hf	-795.43	kJ/mol	Joback Method
hfus	61.10	kJ/mol	Joback Method
hvap	86.70	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.686		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
rinpol	2762.00		NIST Webbook
tb	901.82	K	Joback Method
tc	1104.14	K	Joback Method
tf	483.76	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.27	J/mol×K	901.82	Joback Method
cpg	1180.24	J/mol×K	935.54	Joback Method
cpg	1198.01	J/mol×K	969.26	Joback Method
cpg	1214.61	J/mol×K	1002.98	Joback Method
cpg	1230.09	J/mol×K	1036.70	Joback Method
cpg	1244.52	J/mol×K	1070.42	Joback Method
cpg	1257.93	J/mol×K	1104.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348914&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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